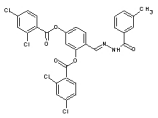


ID: ST097994

Formula: C29H18Cl4N2O5

MW: 616.28

LogP: 9.01

LogS: -7.19

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 4-{(1E)-2-[(3-methylphenyl)carbonylamino]-2-azavinyl}-3-(2,4-dichlorophenylcar bonyloxy

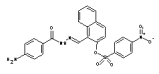
Rotation Bonds: 8

Lipinski: 2

N+O: 7

Chiral Centers: 0

Smiles: c1(C(Oc2c(/C=N\NC(c3cc(C)ccc3)=O)ccc(OC(c3c(cc(cc3)Cl)Cl)=O)c2)=O)c(cc(cc1)Cl)Cl



ID: ST097995

Formula: C24H18N4O6S

MW: 490.5

LogP: 3.71

LogS: -5.11

Acceptors: 6

Donors: 3

Oil: SOLID

IUPACNAME: 1-{(1E)-2-[(4-aminophenyl)carbonylamino]-2-azavinyl}-2-naphthyl 4-nitrobenzene sulfonat

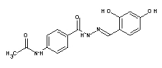
Rotation Bonds: 3

Lipinski: 4

N+O: 10

Chiral Centers: 0

Smiles: S(Oc1c(c2ccccc2cc1)/C=N\NC(c1ccc(cc1)N)=O)(c1ccc([N+]([O-])=O)cc1)(=O)=O



ID: ST097996

Formula: C16H15N3O4

MW: 313.31

LogP: 1.31

LogS: -3.36

Acceptors: 4

Donors: 4

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2,4-dihydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)acetamide

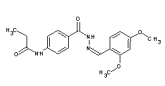
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)C)cc1)(N\N=C\c1c(cc(cc1)O)O)=O



ID: ST097997

Formula: C19H21N3O4

MW: 355.39

LogP: 2.82

LogS: -4.27

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-(4-{N-[(1Z)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)propanamide

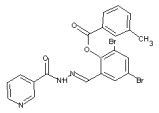
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)CC)cc1)(N\N=C/c1c(cc(cc1)OC)OC)=O



ID: ST097998

Formula: C21H15Br2N3O3

MW: 517.18

LogP: 5.14

LogS: -5.35

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(3-pyridylcarbonylamino)-2-azavinyl]-4,6-dibromophenyl 3-methylbenzo ate

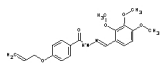
Rotation Bonds: 5

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: c1(OC(c2cc(C)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(c1ncccc1)=O



ID: ST097999

Formula: C20H22N2O5

MW: 370.41

LogP: 3.68

LogS: -4.66

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3,4-trimethoxyphenyl)-1-azavinyl](4-prop-2-enyloxyphenyl)carboxam ide

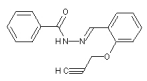
Rotation Bonds: 6

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: c1(c(c(/C=N\NC(c2ccc(cc2)OCC=C)=O)ccc1OC)OC)OC



ID: ST098000

Formula: C17H14N2O2

MW: 278.31

LogP: 3.72

LogS: -4.3

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-prop-2-ynyloxyphenyl)-1-azavinyl]benzamide

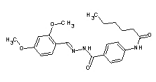
Rotation Bonds: 4

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(N\N=C\c1c(OCC#C)cccc1)(=O)c1ccccc1



ID: ST098001

Formula: C22H27N3O4

MW: 397.47

LogP: 4.31

LogS: -4.96

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)hexanamide

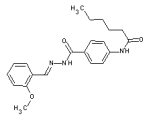
Rotation Bonds: 8

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)CCCCC)cc1)(N\N=C\c1c(cc(cc1)OC)OC)=O



ID: ST098002

Formula: C21H25N3O3

MW: 367.45

LogP: 4.43

LogS: -4.88

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)hexanamide

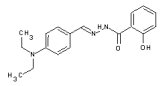
Rotation Bonds: 7

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)CCCCC)cc1)(N\N=C\c1c(OC)cccc1)=O



ID: ST098003

Formula: C18H21N3O2

MW: 311.38

LogP: 4.24

LogS: -4.57

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-{(1E)-2-[4-(diethylamino)phenyl]-1-azavinyl}(2-hydroxyphenyl)carboxamide

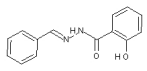
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2ccc(cc2)N(CC)CC)=O)c(O)cccc1



ID: ST098004

Formula: C14H12N2O2

MW: 240.26

LogP: 3.06

LogS: -3.8

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-((1E)-2-phenyl-1-azavinyl)(2-hydroxyphenyl)carboxamide

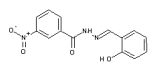
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2ccccc2)=O)c(O)cccc1



ID: ST098005

Formula: C14H11N3O4

MW: 285.26

LogP: 2.53

LogS: -3.74

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl](3-nitrophenyl)carboxamide

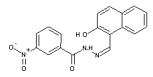
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1cc(C(N\N=C\c2c(O)cccc2)=O)ccc1)([O-])=O



ID: ST098006

Formula: C18H13N3O4

MW: 335.32

LogP: 3.74

LogS: -4.42

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1Z)-2-(2-hydroxynaphthyl)-1-azavinyl](3-nitrophenyl)carboxamide

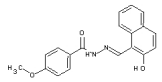
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1cc(C(N\N=C/c2c3c(cccc3)ccc2O)=O)ccc1)([O-])=O



ID: ST098007

Formula: C19H16N2O3

MW: 320.35

LogP: 3.8

LogS: -4.46

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxynaphthyl)-1-azavinyl](4-methoxyphenyl)carboxamide

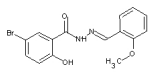
Rotation Bonds: 2

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(c2c(cccc2)ccc1O)/C=N\NC(c1ccc(cc1)OC)=O



ID: ST098008

Formula: C15H13BrN2O3

MW: 349.18

LogP: 3.4

LogS: -4.14

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-methoxyphenyl)-1-azavinyl](5-bromo-2-hydroxyphenyl)carboxamide

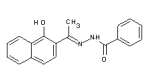
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2c(OC)cccc2)=O)c(ccc(c1)Br)O



ID: ST098009

Formula: C19H16N2O2

MW: 304.35

LogP: 4.3

LogS: -4.54

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(1-hydroxy(2-naphthyl))-1-azaprop-1-enyl]benzamide

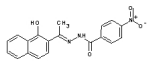
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(c2ccccc2cc1)O)/C(=N\NC(=O)c1ccccc1)C



ID: ST098010

Formula: C19H15N3O4

MW: 349.35

LogP: 4.04

LogS: -4.56

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(1-hydroxy(2-naphthyl))-1-azaprop-1-enyl](4-nitrophenyl)carboxamide

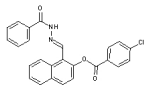
Rotation Bonds: 3

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1ccc(C(N\N=C(\c2c(c3ccccc3cc2)O)C)=O)cc1)([O-])=O



ID: ST098011

Formula: C25H17ClN2O3

MW: 428.87

LogP: 6.82

LogS: -5.96

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 1-[(1E)-2-(phenylcarbonylamino)-2-azavinyl]-2-naphthyl 4-chlorobenzoate

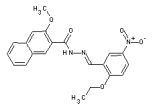
Rotation Bonds: 3

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: c1(c(OC(c2ccc(cc2)Cl)=O)ccc2c1cccc2)/C=N\NC(=O)c1ccccc1



ID: ST098012

Formula: C21H19N3O5

MW: 393.4

LogP: 4.39

LogS: -5

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-ethoxy-5-nitrophenyl)-1-azavinyl](3-methoxy(2-naphthyl))carboxami de

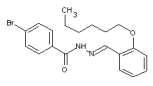
Rotation Bonds: 6

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: c1(cc2ccccc2cc1OC)C(N\N=C\c1cc([N+]([O-])=O)ccc1OCC)=O



ID: ST098013

Formula: C20H23BrN2O2

MW: 403.32

LogP: 6.45

LogS: -5.52

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hexyloxyphenyl)-1-azavinyl](4-bromophenyl)carboxamide

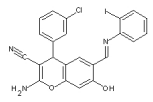
Rotation Bonds: 8

Lipinski: 3

N+O: 4

Chiral Centers: 0

Smiles: C(c1ccc(cc1)Br)(N\N=C\c1c(OCCCCCC)cccc1)=O



ID: ST098014

Formula: C23H15ClIN3O2

MW: 527.75

LogP: 6.2

LogS: -5.71

Acceptors: 2

Donors: 3

Oil: SOLID

IUPACNAME: 6-[(1E)-2-(2-iodophenyl)-2-azavinyl]-2-amino-4-(3-chlorophenyl)-7-hydroxy-4H-c hromene

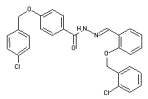
Rotation Bonds: 3

Lipinski: 2

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1cc(Cl)ccc1)cc(c(O)c2)/C=N\c1c(I)cccc1)N)C#N



ID: ST098015

Formula: C28H22Cl2N2O3

MW: 505.4

LogP: 8.1

LogS: -6.63

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-((1E)-2-{2-[(2-chlorophenyl)methoxy]phenyl}-1-azavinyl){4-[(4-chlorophenyl)m ethoxy]p

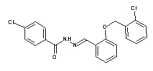
Rotation Bonds: 6

Lipinski: 2

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(OCc2ccc(cc2)Cl)cc1)(N\N=C\c1c(OCc2c(Cl)cccc2)cccc1)=O



ID: ST098016

Formula: C21H16Cl2N2O2

MW: 399.28

LogP: 6.02

LogS: -5.46

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-((1E)-2-{2-[(2-chlorophenyl)methoxy]phenyl}-1-azavinyl)(4-chlorophenyl)carbo xamide

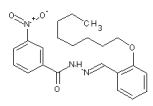
Rotation Bonds: 5

Lipinski: 3

N+O: 4

Chiral Centers: 0

Smiles: C(c1ccc(cc1)Cl)(N\N=C\c1c(OCc2c(Cl)cccc2)cccc1)=O



ID: ST098017

Formula: C22H27N3O4

MW: 397.47

LogP: 6.52

LogS: -5.69

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-octyloxyphenyl)-1-azavinyl](3-nitrophenyl)carboxamide

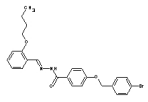
Rotation Bonds: 11

Lipinski: 3

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1cc(C(N\N=C\c2c(OCCCCCCCC)cccc2)=O)ccc1)([O-])=O



ID: ST098018

Formula: C25H25BrN2O3

MW: 481.39

LogP: 7.53

LogS: -6.22

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-butoxyphenyl)-1-azavinyl]{4-[(4-bromophenyl)methoxy]phenyl}carbox amide

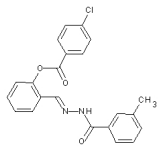
Rotation Bonds: 7

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(OCc2ccc(cc2)Br)cc1)(N\N=C\c1c(OCCCC)cccc1)=O



ID: ST098019

Formula: C22H17ClN2O3

MW: 392.84

LogP: 6.09

LogS: -5.51

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(3-methylphenyl)carbonylamino]-2-azavinyl}phenyl 4-chlorobenzoate

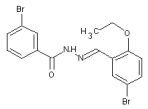
Rotation Bonds: 4

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: C(Oc1c(/C=N\NC(c2cc(C)ccc2)=O)cccc1)(c1ccc(cc1)Cl)=O



ID: ST098020

Formula: C16H14Br2N2O2

MW: 426.11

LogP: 5.01

LogS: -4.88

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-ethoxyphenyl)-1-azavinyl](3-bromophenyl)carboxamide

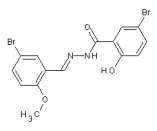
Rotation Bonds: 5

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(Br)ccc1)(N\N=C\c1c(ccc(c1)Br)OCC)=O



ID: ST098021

Formula: C15H12Br2N2O3

MW: 428.08

LogP: 4.04

LogS: -4.44

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl](5-bromo-2-hydroxyphenyl)carbox amid

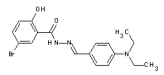
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2c(ccc(c2)Br)OC)=O)c(ccc(c1)Br)O



ID: ST098022

Formula: C18H20BrN3O2

MW: 390.28

LogP: 4.76

LogS: -4.84

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-{(1E)-2-[4-(diethylamino)phenyl]-1-azavinyl}(5-bromo-2-hydroxyphenyl)carboxa mide

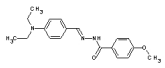
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2ccc(cc2)N(CC)CC)=O)c(ccc(c1)Br)O



ID: ST098023

Formula: C19H23N3O2

MW: 325.41

LogP: 4.37

LogS: -4.79

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[4-(diethylamino)phenyl]-1-azavinyl}(4-methoxyphenyl)carboxamide

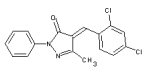
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(cc1)OC)(N\N=C\c1ccc(cc1)N(CC)CC)=O



ID: ST098024

Formula: C17H12Cl2N2O

MW: 331.2

LogP: 5.06

LogS: -4.97

Acceptors: 1

Donors: 0

Oil: SOLID

IUPACNAME: 4-[(2,4-dichlorophenyl)methylene]-3-methyl-1-phenyl-1,2-diazolin-5-one

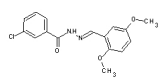
Rotation Bonds: 1

Lipinski: 4

N+O: 3

Chiral Centers: 0

Smiles: C1(/C(N(c2ccccc2)N=C1C)=O)=C\c1c(cc(cc1)Cl)Cl



ID: ST098025

Formula: C16H15ClN2O3

MW: 318.76

LogP: 3.57

LogS: -4.35

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,5-dimethoxyphenyl)-1-azavinyl](3-chlorophenyl)carboxamide

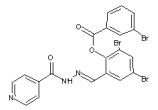
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1cc(Cl)ccc1)(N\N=C\c1c(ccc(c1)OC)OC)=O



ID: ST098026

Formula: C20H12Br3N3O3

MW: 582.05

LogP: 5.28

LogS: -5.43

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(4-pyridylcarbonylamino)-2-azavinyl]-4,6-dibromophenyl 3-bromobenzoa te

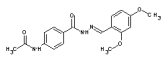
Rotation Bonds: 4

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: c1(OC(c2cc(Br)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(=O)c1ccncc1



ID: ST098027

Formula: C18H19N3O4

MW: 341.37

LogP: 1.98

LogS: -3.97

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)acetamide

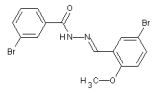
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)C)cc1)(N\N=C\c1c(cc(cc1)OC)OC)=O



ID: ST098028

Formula: C15H12Br2N2O2

MW: 412.08

LogP: 4.43

LogS: -4.62

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl](3-bromophenyl)carboxamide

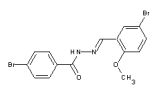
Rotation Bonds: 4

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(Br)ccc1)(N\N=C\c1c(ccc(c1)Br)OC)=O



ID: ST098029

Formula: C15H12Br2N2O2

MW: 412.08

LogP: 4.51

LogS: -4.64

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl](4-bromophenyl)carboxamide

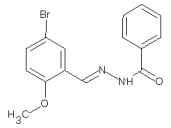
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(ccc(c1)Br)OC)/C=N\NC(c1ccc(cc1)Br)=O



ID: ST098030

Formula: C15H13BrN2O2

MW: 333.18

LogP: 3.88

LogS: -4.35

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl]benzamide

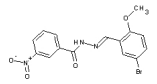
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(ccc(c1)Br)OC)/C=N\NC(=O)c1ccccc1



ID: ST098031

Formula: C15H12BrN3O4

MW: 378.18

LogP: 3.58

LogS: -4.35

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl](3-nitrophenyl)carboxamide

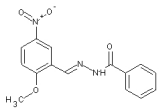
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1cc(C(N\N=C\c2c(ccc(c2)Br)OC)=O)ccc1)([O-])=O



ID: ST098032

Formula: C15H13N3O4

MW: 299.29

LogP: 2.81

LogS: -4.01

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-methoxy-5-nitrophenyl)-1-azavinyl]benzamide

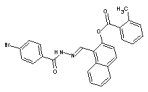
Rotation Bonds: 2

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1cc(/C=N\NC(=O)c2ccccc2)c(cc1)OC)([O-])=O



ID: ST098033

Formula: C26H19BrN2O3

MW: 487.35

LogP: 7.52

LogS: -6.28

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 1-{(1E)-2-[(4-bromophenyl)carbonylamino]-2-azavinyl}-2-naphthyl 2-methylbenzoa te

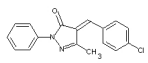
Rotation Bonds: 4

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: C(Oc1c(c2ccccc2cc1)/C=N\NC(c1ccc(cc1)Br)=O)(c1c(C)cccc1)=O



ID: ST098034

Formula: C17H13ClN2O

MW: 296.76

LogP: 4.52

LogS: -4.72

Acceptors: 1

Donors: 0

Oil: SOLID

IUPACNAME: 4-[(4-chlorophenyl)methylene]-3-methyl-1-phenyl-1,2-diazolin-5-one

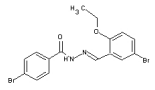
Rotation Bonds: 0

Lipinski: 4

N+O: 3

Chiral Centers: 0

Smiles: C1(/C(N(c2ccccc2)N=C1C)=O)=C\c1ccc(cc1)Cl



ID: ST098035

Formula: C16H14Br2N2O2

MW: 426.11

LogP: 5.09

LogS: -4.9

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-ethoxyphenyl)-1-azavinyl](4-bromophenyl)carboxamide

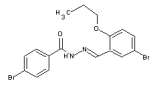
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(ccc(c1)Br)OCC)/C=N\NC(c1ccc(cc1)Br)=O



ID: ST098036

Formula: C17H16Br2N2O2

MW: 440.13

LogP: 5.59

LogS: -5.13

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-propoxyphenyl)-1-azavinyl](4-bromophenyl)carboxamide

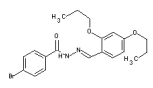
Rotation Bonds: 4

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(ccc(c1)Br)OCCC)/C=N\NC(c1ccc(cc1)Br)=O



ID: ST098037

Formula: C20H23BrN2O3

MW: 419.32

LogP: 5.9

LogS: -5.39

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-dipropoxyphenyl)-1-azavinyl](4-bromophenyl)carboxamide

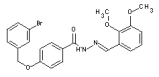
Rotation Bonds: 8

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(cc1)Br)(N\N=C\c1c(cc(cc1)OCCC)OCCC)=O



ID: ST098038

Formula: C23H21BrN2O4

MW: 469.33

LogP: 5.73

LogS: -5.54

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3-dimethoxyphenyl)-1-azavinyl]{4-[(3-bromophenyl)methoxy]phenyl}c arboxa

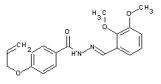
Rotation Bonds: 6

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(OCc2cc(Br)ccc2)cc1)(N\N=C\c1c(c(OC)ccc1)OC)=O



ID: ST098039

Formula: C19H20N2O4

MW: 340.38

LogP: 3.74

LogS: -4.57

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3-dimethoxyphenyl)-1-azavinyl](4-prop-2-enyloxyphenyl)carboxamide

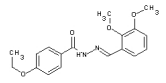
Rotation Bonds: 6

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(cc1)OCC=C)(N\N=C\c1c(c(OC)ccc1)OC)=O



ID: ST098040

Formula: C18H20N2O4

MW: 328.37

LogP: 3.24

LogS: -4.35

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3-dimethoxyphenyl)-1-azavinyl](4-ethoxyphenyl)carboxamide

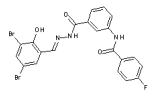
Rotation Bonds: 5

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(cc1)OCC)(N\N=C\c1c(c(OC)ccc1)OC)=O



ID: ST098041

Formula: C21H14Br2FN3O3

MW: 535.17

LogP: 4.84

LogS: -5.03

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(3,5-dibromo-2-hydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-f luoroph

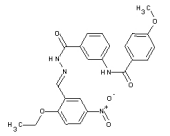
Rotation Bonds: 4

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(c(Br)cc(c2)Br)O)=O)ccc1)(c1ccc(cc1)F)=O



ID: ST098042

Formula: C24H22N4O6

MW: 462.46

LogP: 4.3

LogS: -5.14

Acceptors: 6

Donors: 2

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-ethoxy-5-nitrophenyl)-1-azavinyl]carbamoyl}phenyl)(4-methox yphenyl)

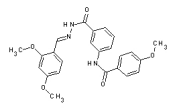
Rotation Bonds: 4

Lipinski: 4

N+O: 10

Chiral Centers: 0

Smiles: [N+](c1cc(/C=N\NC(c2cc(NC(c3ccc(cc3)OC)=O)ccc2)=O)c(cc1)OCC)([O-])=O



ID: ST098043

Formula: C24H23N3O5

MW: 433.46

LogP: 4.03

LogS: -5

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-methoxyph enyl)c

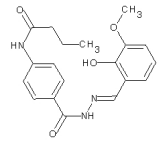
Rotation Bonds: 5

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(cc(cc2)OC)OC)=O)ccc1)(c1ccc(cc1)OC)=O



ID: ST098044

Formula: C19H21N3O4

MW: 355.39

LogP: 3.09

LogS: -4.2

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)butana mide

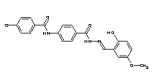
Rotation Bonds: 6

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)CCC)cc1)(N\N=C\c1c(c(OC)ccc1)O)=O



ID: ST098045

Formula: C22H18ClN3O4

MW: 423.86

LogP: 4.12

LogS: -4.81

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-hydroxy-5-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-chl orophe

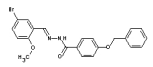
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(Nc1ccc(C(N\N=C\c2c(ccc(c2)OC)O)=O)cc1)(c1ccc(cc1)Cl)=O



ID: ST098046

Formula: C22H19BrN2O3

MW: 439.31

LogP: 5.77

LogS: -5.45

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-methoxyphenyl)-1-azavinyl][4-(phenylmethoxy)phenyl]carbox amide

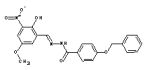
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(c(ccc(c1)Br)OC)/C=N\NC(c1ccc(OCc2ccccc2)cc1)=O



ID: ST098047

Formula: C22H19N3O6

MW: 421.41

LogP: 4.54

LogS: -5.04

Acceptors: 6

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-5-methoxy-3-nitrophenyl)-1-azavinyl][4-(phenylmethoxy)phe nyl]carb

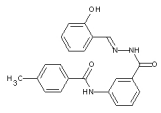
Rotation Bonds: 4

Lipinski: 4

N+O: 9

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)c(c(/C=N\NC(c2ccc(OCc3ccccc3)cc2)=O)cc(c1)OC)O



ID: ST098048

Formula: C22H19N3O3

MW: 373.41

LogP: 4.4

LogS: -4.77

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-methylphenyl) carboxa

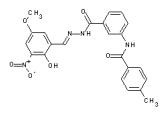
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(O)cccc2)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098049

Formula: C23H20N4O6

MW: 448.44

LogP: 4.22

LogS: -4.97

Acceptors: 6

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-hydroxy-5-methoxy-3-nitrophenyl)-1-azavinyl]carbamoyl}pheny l)(4-me

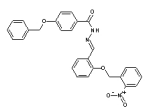
Rotation Bonds: 4

Lipinski: 4

N+O: 10

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)c(c(/C=N\NC(c2cc(NC(c3ccc(cc3)C)=O)ccc2)=O)cc(c1)OC)O



ID: ST098050

Formula: C28H23N3O5

MW: 481.51

LogP: 6.71

LogS: -6.14

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-((1E)-2-{2-[(2-nitrophenyl)methoxy]phenyl}-1-azavinyl)[4-(phenylmethoxy)phen yl]carbo

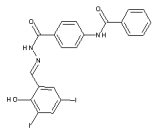
Rotation Bonds: 5

Lipinski: 3

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1c(COc2c(/C=N\NC(c3ccc(OCc4ccccc4)cc3)=O)cccc2)cccc1)([O-])=O



ID: ST098051

Formula: C21H15I2N3O3

MW: 611.18

LogP: 6.69

LogS: -5.77

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-hydroxy-3,5-diiodophenyl)-1-azavinyl]carbamoyl}phenyl)benza mide

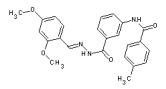
Rotation Bonds: 3

Lipinski: 2

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1ccc(C(N\N=C\c2c(c(I)cc(c2)I)O)=O)cc1)(=O)c1ccccc1



ID: ST098052

Formula: C24H23N3O4

MW: 417.46

LogP: 4.7

LogS: -5.17

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-methylphe nyl)car

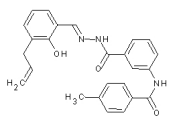
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(cc(cc2)OC)OC)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098053

Formula: C25H23N3O3

MW: 413.48

LogP: 5.5

LogS: -5.38

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-hydroxy-3-prop-2-enylphenyl)-1-azavinyl]carbamoyl}phenyl)(4 -methylp

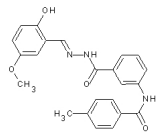
Rotation Bonds: 6

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(c(CC=C)ccc2)O)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098054

Formula: C23H21N3O4

MW: 403.44

LogP: 4.22

LogS: -4.84

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-hydroxy-5-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-met hylphe

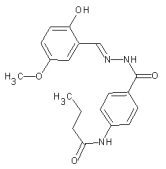
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(ccc(c2)OC)O)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098055

Formula: C19H21N3O4

MW: 355.39

LogP: 2.84

LogS: -4.17

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-hydroxy-5-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)butana mide

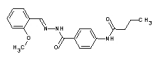
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: c1(c(ccc(c1)OC)O)/C=N\NC(c1ccc(NC(=O)CCC)cc1)=O



ID: ST098056

Formula: C19H21N3O3

MW: 339.39

LogP: 3.44

LogS: -4.42

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)butanamide

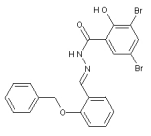
Rotation Bonds: 5

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(NC(=O)CCC)cc1)(N\N=C\c1c(OC)cccc1)=O



ID: ST098057

Formula: C21H16Br2N2O3

MW: 504.18

LogP: 5.37

LogS: -5.23

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-{(1E)-2-[2-(phenylmethoxy)phenyl]-1-azavinyl}(3,5-dibromo-2-hydroxyphenyl)ca rboxam

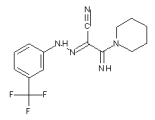
Rotation Bonds: 6

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: c1(c(c(Br)cc(c1)Br)O)C(N\N=C\c1c(OCc2ccccc2)cccc1)=O



ID: ST098058

Formula: C15H16F3N5

MW: 323.32

LogP: 2.64

LogS: -3.9

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminopiperidylmethyl)-3-{[3-(trifluoromethyl)phenyl]amino}-3-azaprop-2 -enenitrile

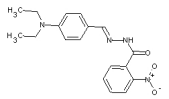
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(C(F)(F)F)ccc1)C#N)(N1CCCCC1)=N



ID: ST098059

Formula: C18H20N4O3

MW: 340.38

LogP: 4.24

LogS: -4.74

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[4-(diethylamino)phenyl]-1-azavinyl}(2-nitrophenyl)carboxamide

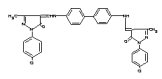
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1c(C(N\N=C\c2ccc(cc2)N(CC)CC)=O)cccc1)([O-])=O



ID: ST098060

Formula: C34H26Cl2N6O2

MW: 621.53

LogP: 6.81

LogS: -6.83

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: 1-(4-chlorophenyl)-4-[({4-[4-({[1-(4-chlorophenyl)-3-methyl-5-oxo(1,2-diazolin -4-ylidene)]r

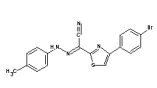
Rotation Bonds: 0

Lipinski: 2

N+O: 8

Chiral Centers: 0

Smiles: N1(N=C(C)C(/C1=O)=C/Nc1ccc(cc1)c1ccc(N\C=C2\C(N(c3ccc(cc3)Cl)N=C2C)=O)cc1)c1ccc(cc



ID: ST098061

Formula: C18H13BrN4S

MW: 397.3

LogP: 5.04

LogS: -5.01

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-bromophenyl)(1,3-thiazol-2-yl)]-3-[(4-methylphenyl)amino]-3-azapr op-2-ener

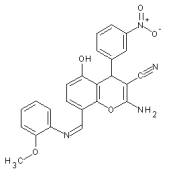
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)C)C#N)scc1c1ccc(cc1)Br



ID: ST098062

Formula: C24H18N4O5

MW: 442.43

LogP: 4.11

LogS: -4.99

Acceptors: 5

Donors: 3

Oil: SOLID

IUPACNAME: 8-[(1Z)-2-(2-methoxyphenyl)-2-azavinyl]-2-amino-5-hydroxy-4-(3-nitrophenyl)-4H -chrome

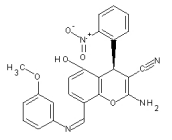
Rotation Bonds: 4

Lipinski: 4

N+O: 9

Chiral Centers: 1

Smiles: C=1(C(c2c(ccc(c2OC1N)/C=N/c1c(OC)cccc1)O)c1cc([N+]([O-])=O)ccc1)C#N



ID: ST098063

Formula: C24H18N4O5

MW: 442.43

LogP: 4.26

LogS: -5.04

Acceptors: 5

Donors: 3

Oil: SOLID

IUPACNAME: (4R)-8-[(1Z)-2-(3-methoxyphenyl)-2-azavinyl]-2-amino-5-hydroxy-4-(2-nitropheny l)-4H-ch

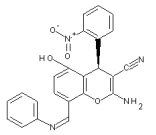
Rotation Bonds: 3

Lipinski: 4

N+O: 9

Chiral Centers: 1

Smiles: C=1([C@@H](c2c(ccc(c2OC1N)/C=N/c1cc(OC)ccc1)O)c1c([N+]([O-])=O)cccc1)C#N



ID: ST098064

Formula: C23H16N4O4

MW: 412.4

LogP: 4.34

LogS: -4.95

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: (4R)-8-((1Z)-2-phenyl-2-azavinyl)-2-amino-5-hydroxy-4-(2-nitrophenyl)-4H-chrom ene-3-c

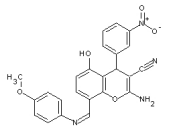
Rotation Bonds: 2

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: C=1([C@@H](c2c(ccc(c2OC1N)/C=N/c1ccccc1)O)c1c([N+]([O-])=O)cccc1)C#N



ID: ST098065

Formula: C24H18N4O5

MW: 442.43

LogP: 4.06

LogS: -4.99

Acceptors: 5

Donors: 3

Oil: SOLID

IUPACNAME: 8-[(1Z)-2-(4-methoxyphenyl)-2-azavinyl]-2-amino-5-hydroxy-4-(3-nitrophenyl)-4H -chrome

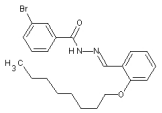
Rotation Bonds: 3

Lipinski: 4

N+O: 9

Chiral Centers: 1

Smiles: C=1(C(c2c(ccc(c2OC1N)/C=N/c1ccc(cc1)OC)O)c1cc([N+]([O-])=O)ccc1)C#N



ID: ST098066

Formula: C22H27BrN2O2

MW: 431.37

LogP: 7.36

LogS: -5.97

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-octyloxyphenyl)-1-azavinyl](3-bromophenyl)carboxamide

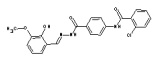
Rotation Bonds: 11

Lipinski: 3

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(Br)ccc1)(N\N=C\c1c(OCCCCCCCCC)cccc1)=O



ID: ST098067

Formula: C22H18ClN3O4

MW: 423.86

LogP: 4.36

LogS: -4.84

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl]carbamoyl}phenyl)(2-chl orophe

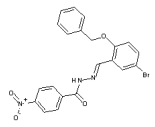
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1c(Cl)cccc1)(Nc1ccc(C(N\N=C\c2c(c(OC)ccc2)O)=O)cc1)=O



ID: ST098068

Formula: C21H16BrN3O4

MW: 454.28

LogP: 5.28

LogS: -5.29

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[5-bromo-2-(phenylmethoxy)phenyl]-1-azavinyl}(4-nitrophenyl)carboxam ide

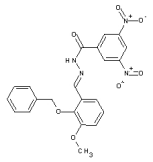
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: [N+](c1ccc(C(N\N=C\c2c(OCc3ccccc3)ccc(c2)Br)=O)cc1)([O-])=O



ID: ST098069

Formula: C22H18N4O7

MW: 450.41

LogP: 4.66

LogS: -5.18

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[3-methoxy-2-(phenylmethoxy)phenyl]-1-azavinyl}(3,5-dinitrophenyl)ca rboxami

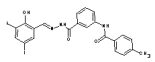
Rotation Bonds: 5

Lipinski: 4

N+O: 11

Chiral Centers: 0

Smiles: [N+](c1cc([N+]([O-])=O)cc(c1)C(N\N=C\c1c(OCc2ccccc2)c(OC)ccc1)=O)([O-])=O



ID: ST098070

Formula: C22H17I2N3O3

MW: 625.2

LogP: 7.2

LogS: -6

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2-hydroxy-3,5-diiodophenyl)-1-azavinyl]carbamoyl}phenyl)(4-me thylphe

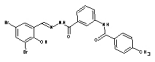
Rotation Bonds: 4

Lipinski: 2

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(c(I)cc(c2)I)O)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098071

Formula: C22H17Br2N3O3

MW: 531.2

LogP: 5.45

LogS: -5.28

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(3,5-dibromo-2-hydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)(4-m ethylph

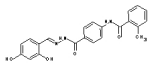
Rotation Bonds: 4

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: C(Nc1cc(C(N\N=C\c2c(c(Br)cc(c2)Br)O)=O)ccc1)(c1ccc(cc1)C)=O



ID: ST098072

Formula: C22H19N3O4

MW: 389.41

LogP: 3.94

LogS: -4.53

Acceptors: 4

Donors: 4

Oil: SOLID

IUPACNAME: N-(4-{N-[(1E)-2-(2,4-dihydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)(2-methylphe nyl)carb

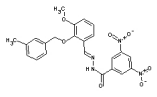
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(Nc1ccc(C(N\N=C\c2c(cc(cc2)O)O)=O)cc1)(c1c(C)cccc1)=O



ID: ST098073

Formula: C23H20N4O7

MW: 464.43

LogP: 5.21

LogS: -5.43

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: N-((1E)-2-{3-methoxy-2-[(3-methylphenyl)methoxy]phenyl}-1-azavinyl)(3,5-dinitr ophenyl)

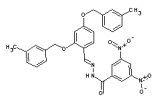
Rotation Bonds: 6

Lipinski: 4

N+O: 11

Chiral Centers: 0

Smiles: [N+](c1cc([N+]([O-])=O)cc(c1)C(N\N=C\c1c(OCc2cc(C)ccc2)c(OC)ccc1)=O)([O-])=O



ID: ST098074

Formula: C30H26N4O7

MW: 554.56

LogP: 7.54

LogS: -6.64

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: N-((1E)-2-{2,4-bis[(3-methylphenyl)methoxy]phenyl}-1-azavinyl)(3,5-dinitrophen yl)carbox

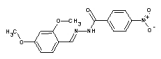
Rotation Bonds: 8

Lipinski: 2

N+O: 11

Chiral Centers: 0

Smiles: [N+](c1cc([N+]([O-])=O)cc(c1)C(N\N=C\c1c(cc(cc1)OCc1cc(C)ccc1)OCc1cc(C)ccc1)=O)([O-])=O



ID: ST098075

Formula: C16H15N3O5

MW: 329.31

LogP: 2.86

LogS: -4.14

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl](4-nitrophenyl)carboxamide

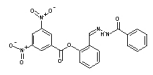
Rotation Bonds: 4

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1ccc(C(N\N=C\c2c(cc(cc2)OC)OC)=O)cc1)([O-])=O



ID: ST098076

Formula: C21H14N4O7

MW: 434.36

LogP: 4.73

LogS: -5.12

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1Z)-2-(phenylcarbonylamino)-2-azavinyl]phenyl 3,5-dinitrobenzoate

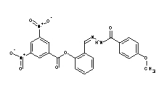
Rotation Bonds: 3

Lipinski: 4

N+O: 11

Chiral Centers: 0

Smiles: [N+](c1cc([N+]([O-])=O)cc(C(Oc2c(/C=N/NC(=O)c3ccccc3)cccc2)=O)c1)([O-])=O



ID: ST098077

Formula: C22H16N4O8

MW: 464.39

LogP: 4.49

LogS: -5.16

Acceptors: 8

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1Z)-2-[(4-methoxyphenyl)carbonylamino]-2-azavinyl}phenyl 3,5-dinitrobenzoa te

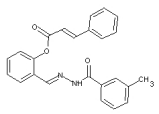
Rotation Bonds: 3

Lipinski: 4

N+O: 12

Chiral Centers: 0

Smiles: [N+](c1cc([N+]([O-])=O)cc(C(Oc2c(/C=N/NC(c3ccc(cc3)OC)=O)cccc2)=O)c1)([O-])=O



ID: ST098078

Formula: C24H20N2O3

MW: 384.43

LogP: 5.95

LogS: -5.54

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(3-methylphenyl)carbonylamino]-2-azavinyl}phenyl (2E)-3-phenylprop- 2-enoat

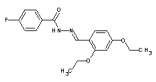
Rotation Bonds: 6

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1cc(C)ccc1)(N\N=C\c1c(OC(/C=C\c2ccccc2)=O)cccc1)=O



ID: ST098079

Formula: C18H19FN2O3

MW: 330.36

LogP: 4.02

LogS: -4.57

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-diethoxyphenyl)-1-azavinyl](4-fluorophenyl)carboxamide

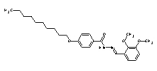
Rotation Bonds: 6

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(cc1)F)(N\N=C\c1c(cc(cc1)OCC)OCC)=O



ID: ST098080

Formula: C26H36N2O4

MW: 440.58

LogP: 7.38

LogS: -6.24

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3-dimethoxyphenyl)-1-azavinyl](4-decyloxyphenyl)carboxamide

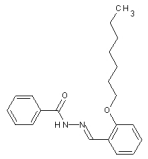
Rotation Bonds: 13

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(cc1)OCCCCCCCCCC)(N\N=C\c1c(c(OC)ccc1)OC)=O



ID: ST098081

Formula: C21H26N2O2

MW: 338.45

LogP: 6.32

LogS: -5.46

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-heptyloxyphenyl)-1-azavinyl]benzamide

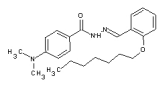
Rotation Bonds: 9

Lipinski: 3

N+O: 4

Chiral Centers: 0

Smiles: C(N\N=C\c1c(OCCCCCCC)cccc1)(=O)c1ccccc1



ID: ST098082

Formula: C23H31N3O2

MW: 381.52

LogP: 6.59

LogS: -5.79

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-heptyloxyphenyl)-1-azavinyl][4-(dimethylamino)phenyl]carboxamide

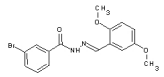
Rotation Bonds: 9

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(cc1)N(C)C)(N\N=C\c1c(OCCCCCCC)cccc1)=O



ID: ST098083

Formula: C16H15BrN2O3

MW: 363.21

LogP: 3.6

LogS: -4.38

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,5-dimethoxyphenyl)-1-azavinyl](3-bromophenyl)carboxamide

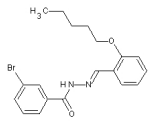
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1cc(Br)ccc1)(N\N=C\c1c(ccc(c1)OC)OC)=O



ID: ST098084

Formula: C19H21BrN2O2

MW: 389.29

LogP: 5.87

LogS: -5.27

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-pentyloxyphenyl)-1-azavinyl](3-bromophenyl)carboxamide

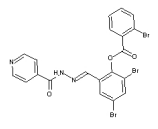
Rotation Bonds: 8

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(Br)ccc1)(N\N=C\c1c(OCCCCC)cccc1)=O



ID: ST098085

Formula: C20H12Br3N3O3

MW: 582.05

LogP: 5.29

LogS: -5.43

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(4-pyridylcarbonylamino)-2-azavinyl]-4,6-dibromophenyl 2-bromobenzoa te

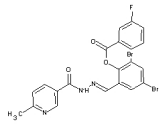
Rotation Bonds: 4

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: C(Oc1c(cc(cc1Br)Br)/C=N\NC(=O)c1ccncc1)(c1c(Br)cccc1)=O



ID: ST098086

Formula: C21H14Br2FN3O3

MW: 535.17

LogP: 5.27

LogS: -5.41

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(6-methyl(3-pyridyl))carbonylamino]-2-azavinyl}-4,6-dibromophenyl 3 -fluorober

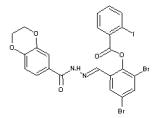
Rotation Bonds: 5

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: c1(OC(c2cc(F)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(c1cnc(cc1)C)=O



ID: ST098087

Formula: C23H15Br2IN2O5

MW: 686.1

LogP: 7.11

LogS: -6.27

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(2H,3H-benzo[3,4-e]1,4-dioxan-6-ylcarbonylamino)-2-azavinyl]-4,6-dib romophe

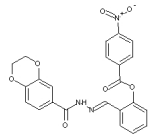
Rotation Bonds: 5

Lipinski: 2

N+O: 7

Chiral Centers: 0

Smiles: C(Oc1c(cc(cc1Br)Br)/C=N\NC(c1cc2OCCOc2cc1)=O)(c1c(I)cccc1)=O



ID: ST098088

Formula: C23H17N3O7

MW: 447.4

LogP: 4.47

LogS: -5.14

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(2H,3H-benzo[3,4-e]1,4-dioxan-6-ylcarbonylamino)-2-azavinyl]phenyl 4 -nitrobe

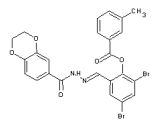
Rotation Bonds: 4

Lipinski: 4

N+O: 10

Chiral Centers: 0

Smiles: [N+](c1ccc(C(Oc2c(/C=N\NC(c3cc4OCCOc4cc3)=O)cccc2)=O)cc1)([O-])=O



ID: ST098089

Formula: C24H18Br2N2O5

MW: 574.23

LogP: 6.55

LogS: -5.97

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(2H,3H-benzo[3,4-e]1,4-dioxan-6-ylcarbonylamino)-2-azavinyl]-4,6-dib romophe

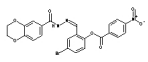
Rotation Bonds: 5

Lipinski: 2

N+O: 7

Chiral Centers: 0

Smiles: c1(OC(c2cc(C)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(c1cc2OCCOc2cc1)=O



ID: ST098090

Formula: C23H16BrN3O7

MW: 526.3

LogP: 5.11

LogS: -5.44

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1Z)-2-(2H,3H-benzo[3,4-e]1,4-dioxan-6-ylcarbonylamino)-2-azavinyl]-4-bromo phenyl

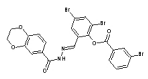
Rotation Bonds: 4

Lipinski: 3

N+O: 10

Chiral Centers: 0

Smiles: [N+](c1ccc(C(Oc2c(cc(cc2)Br)/C=N/NC(c2cc3OCCOc3cc2)=O)=O)cc1)([O-])=O



ID: ST098091

Formula: C23H15Br3N2O5

MW: 639.09

LogP: 6.63

LogS: -6.02

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(2H,3H-benzo[3,4-e]1,4-dioxin-6-ylcarbonylamino)-2-azavinyl]-4,6-dib romopher

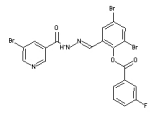
Rotation Bonds: 5

Lipinski: 2

N+O: 7

Chiral Centers: 0

Smiles: c1(OC(c2cc(Br)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(c1cc2OCCOc2cc1)=O



ID: ST098092

Formula: C20H11Br3FN3O3

MW: 600.04

LogP: 5.27

LogS: -5.44

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(5-bromo(3-pyridyl))carbonylamino]-2-azavinyl}-4,6-dibromophenyl 3- fluorober

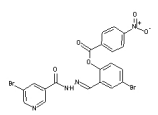
Rotation Bonds: 5

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: c1(OC(c2cc(F)ccc2)=O)c(cc(cc1Br)Br)/C=N\NC(c1cc(Br)cnc1)=O



ID: ST098093

Formula: C20H12Br2N4O5

MW: 548.15

LogP: 4.45

LogS: -5.16

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(5-bromo(3-pyridyl))carbonylamino]-2-azavinyl}-4-bromophenyl 4-nitr obenzoat

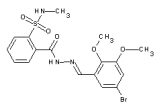
Rotation Bonds: 4

Lipinski: 3

N+O: 9

Chiral Centers: 0

Smiles: [N+](c1ccc(C(Oc2c(cc(cc2)Br)/C=N\NC(c2cc(Br)cnc2)=O)=O)cc1)([O-])=O



ID: ST098094

Formula: C17H18BrN3O5S

MW: 456.32

LogP: 2.71

LogS: -4.4

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2,3-dimethoxyphenyl)-1-azavinyl]{2-[(methylamino)sulfonyl]p henyl}ca

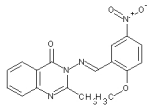
Rotation Bonds: 6

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: S(c1c(C(N\N=C\c2c(c(OC)cc(c2)Br)OC)=O)cccc1)(=O)(=O)NC



ID: ST098095

Formula: C17H14N4O4

MW: 338.32

LogP: 2.03

LogS: -4.09

Acceptors: 4

Donors: 0

Oil: SOLID

IUPACNAME: 3-[(1E)-2-(2-methoxy-5-nitrophenyl)-1-azavinyl]-2-methyl-3-hydroquinazolin-4-o ne

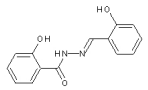
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: n1(c(c2ccccc2nc1C)=O)\N=C\c1cc([N+]([O-])=O)ccc1OC



ID: ST098096

Formula: C14H12N2O3

MW: 256.26

LogP: 2.47

LogS: -3.56

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl](2-hydroxyphenyl)carboxamide

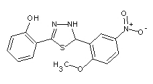
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2c(O)cccc2)=O)c(O)cccc1



ID: ST098097

Formula: C15H13N3O4S

MW: 331.35

LogP: 4.1

LogS: -4.37

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: 2-[2-(2-methoxy-5-nitrophenyl)-1,3,4-thiadiazolin-5-yl]phenol

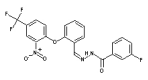
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 1

Smiles: C=1(SC(c2cc([N+]([O-])=O)ccc2OC)NN1)c1c(O)cccc1



ID: ST098098

Formula: C21H13F4N3O4

MW: 447.35

LogP: 5.06

LogS: -5.15

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: N-((1Z)-2-{2-[2-nitro-4-(trifluoromethyl)phenoxy]phenyl}-1-azavinyl)(3-fluorop henyl)carbo

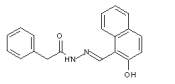
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)c(Oc2c(/C=N/NC(c3cc(F)ccc3)=O)cccc2)ccc(C(F)(F)F)c1



ID: ST098099

Formula: C19H16N2O2

MW: 304.35

LogP: 3.64

LogS: -4.39

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxynaphthyl)-1-azavinyl]-2-phenylacetamide

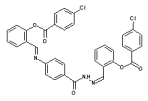
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c2c(cccc2)ccc1O)/C=N\NC(=O)Cc1ccccc1



ID: ST098100

Formula: C35H23Cl2N3O5

MW: 636.49

LogP: 9.5

LogS: -7.65

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[4-(N-{(1Z)-2-[2-(4-chlorophenylcarbonyloxy)phenyl]-1-azavinyl}carba moyl)phe

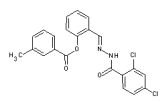
Rotation Bonds: 7

Lipinski: 2

N+O: 8

Chiral Centers: 0

Smiles: C(Oc1c(/C=N\c2ccc(C(N\N=C/c3c(OC(c4ccc(cc4)Cl)=O)cccc3)=O)cc2)cccc1)(c1ccc(cc1)Cl)=O



ID: ST098101

Formula: C22H16Cl2N2O3

MW: 427.29

LogP: 6.45

LogS: -5.7

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(2,4-dichlorophenyl)carbonylamino]-2-azavinyl}phenyl 3-methylbenzoa te

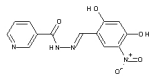
Rotation Bonds: 6

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: c1(c(cc(cc1)Cl)Cl)C(N\N=C\c1c(OC(c2cc(C)ccc2)=O)cccc1)=O



ID: ST098102

Formula: C13H10N4O5

MW: 302.25

LogP: 0.43

LogS: -2.98

Acceptors: 5

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-dihydroxy-5-nitrophenyl)-1-azavinyl]-3-pyridylcarboxamide

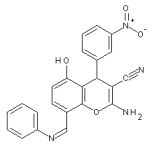
Rotation Bonds: 4

Lipinski: 4

N+O: 9

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)cc(/C=N\NC(c2cnccc2)=O)c(cc1O)O



ID: ST098103

Formula: C23H16N4O4

MW: 412.4

LogP: 4.24

LogS: -4.92

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: 8-((1Z)-2-phenyl-2-azavinyl)-2-amino-5-hydroxy-4-(3-nitrophenyl)-4H-chromene-3 -carbon

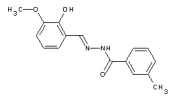
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: C=1(C(c2c(ccc(c2OC1N)/C=N/c1ccccc1)O)c1cc([N+]([O-])=O)ccc1)C#N



ID: ST098104

Formula: C16H16N2O3

MW: 284.31

LogP: 3.39

LogS: -4.05

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl](3-methylphenyl)carboxamide

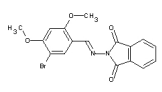
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1cc(C)ccc1)(N\N=C\c1c(c(OC)ccc1)O)=O



ID: ST098105

Formula: C17H13BrN2O4

MW: 389.21

LogP: 0.98

LogS: -3.81

Acceptors: 4

Donors: 0

Oil: SOLID

IUPACNAME: 2-[(1E)-2-(5-bromo-2,4-dimethoxyphenyl)-1-azavinyl]benzo[c]azoline-1,3-dione

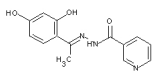
Rotation Bonds: 3

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: N1(C(c2ccccc2C1=O)=O)\N=C\c1c(cc(c(c1)Br)OC)OC



ID: ST098106

Formula: C14H13N3O3

MW: 271.28

LogP: 0.9

LogS: -3.13

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-dihydroxyphenyl)-1-azaprop-1-enyl]-3-pyridylcarboxamide

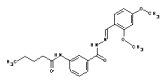
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: c1(c(cc(cc1)O)O)/C(=N\NC(c1cnccc1)=O)C



ID: ST098107

Formula: C21H25N3O4

MW: 383.45

LogP: 3.83

LogS: -4.74

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]carbamoyl}phenyl)pentanamide

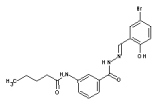
Rotation Bonds: 8

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(c1cc(NC(=O)CCCC)ccc1)(N\N=C\c1c(cc(cc1)OC)OC)=O



ID: ST098108

Formula: C19H20BrN3O3

MW: 418.29

LogP: 4.19

LogS: -4.65

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-(3-{N-[(1E)-2-(5-bromo-2-hydroxyphenyl)-1-azavinyl]carbamoyl}phenyl)pentanam ide

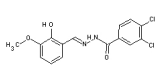
Rotation Bonds: 7

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1cc(NC(=O)CCCC)ccc1)(N\N=C\c1c(ccc(c1)Br)O)=O



ID: ST098109

Formula: C15H12Cl2N2O3

MW: 339.18

LogP: 3.84

LogS: -4.27

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl](3,4-dichlorophenyl)carboxami de

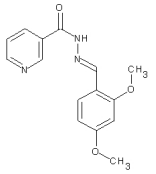
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1cc(Cl)c(cc1)Cl)(N\N=C\c1c(c(OC)ccc1)O)=O



ID: ST098110

Formula: C15H15N3O3

MW: 285.3

LogP: 1.35

LogS: -3.59

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,4-dimethoxyphenyl)-1-azavinyl]-3-pyridylcarboxamide

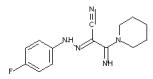
Rotation Bonds: 5

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1cnccc1)(N\N=C\c1c(cc(cc1)OC)OC)=O



ID: ST098111

Formula: C14H16FN5

MW: 273.31

LogP: 2.11

LogS: -3.66

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(4-fluorophenyl)amino]-2-(iminopiperidylmethyl)-3-azaprop-2-enenitrile

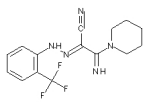
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)F)C#N)(N1CCCCC1)=N



ID: ST098112

Formula: C15H16F3N5

MW: 323.32

LogP: 2.62

LogS: -3.89

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminopiperidylmethyl)-3-{[2-(trifluoromethyl)phenyl]amino}-3-azaprop-2 -enenitrile

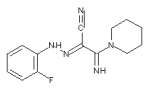
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(C(F)(F)F)cccc1)C#N)(N1CCCCC1)=N



ID: ST098113

Formula: C14H16FN5

MW: 273.31

LogP: 2.02

LogS: -3.62

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(2-fluorophenyl)amino]-2-(iminopiperidylmethyl)-3-azaprop-2-enenitrile

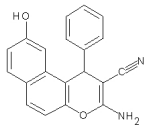
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(F)cccc1)C#N)(N1CCCCC1)=N



ID: ST098114

Formula: C20H14N2O2

MW: 314.34

LogP: 4.12

LogS: -4.52

Acceptors: 2

Donors: 3

Oil: SOLID

IUPACNAME: 3-amino-9-hydroxy-1-phenyl-1H-benzo[f]chromene-2-carbonitrile

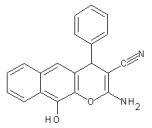
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccccc1)c1c(cc2)ccc(c1)O)N)C#N



ID: ST098115

Formula: C20H14N2O2

MW: 314.34

LogP: 3.95

LogS: -4.45

Acceptors: 2

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-10-hydroxy-4-phenyl-4H-benzo[g]chromene-3-carbonitrile

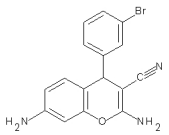
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccccc1)cc1c(cccc1)c2O)N)C#N



ID: ST098116

Formula: C16H12BrN3O

MW: 342.19

LogP: 3.25

LogS: -4.14

Acceptors: 1

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(3-bromophenyl)-4H-chromene-3-carbonitrile

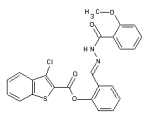
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1cc(Br)ccc1)ccc(N)c2)N)C#N



ID: ST098117

Formula: C24H17ClN2O4S

MW: 464.93

LogP: 6.41

LogS: -5.93

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1E)-2-[(2-methoxyphenyl)carbonylamino]-2-azavinyl}phenyl 3-chlorobenzo[b]t hiopher

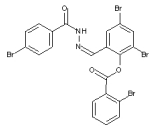
Rotation Bonds: 6

Lipinski: 3

N+O: 6

Chiral Centers: 0

Smiles: c1(sc2ccccc2c1Cl)C(Oc1c(/C=N\NC(c2c(OC)cccc2)=O)cccc1)=O



ID: ST098118

Formula: C21H12Br4N2O3

MW: 659.95

LogP: 7.62

LogS: -6.24

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: 2-{(1Z)-2-[(4-bromophenyl)carbonylamino]-2-azavinyl}-4,6-dibromophenyl 2-bromo benzo

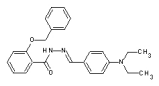
Rotation Bonds: 4

Lipinski: 2

N+O: 5

Chiral Centers: 0

Smiles: C(Oc1c(cc(cc1Br)Br)/C=N/NC(c1ccc(cc1)Br)=O)(c1c(Br)cccc1)=O



ID: ST098119

Formula: C25H27N3O2

MW: 401.51

LogP: 6.09

LogS: -5.74

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[4-(diethylamino)phenyl]-1-azavinyl}[2-(phenylmethoxy)phenyl]carboxa mide

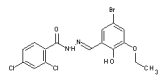
Rotation Bonds: 6

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2ccc(cc2)N(CC)CC)=O)c(OCc2ccccc2)cccc1



ID: ST098120

Formula: C16H13BrCl2N2O3

MW: 432.1

LogP: 4.55

LogS: -4.68

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-3-ethoxy-2-hydroxyphenyl)-1-azavinyl](2,4-dichlorophenyl)ca rboxam

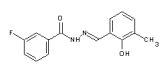
Rotation Bonds: 6

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(c(cc(cc1)Cl)Cl)C(N\N=C\c1c(c(OCC)cc(c1)Br)O)=O



ID: ST098121

Formula: C15H13FN2O2

MW: 272.28

LogP: 3.21

LogS: -3.99

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-3-methylphenyl)-1-azavinyl](3-fluorophenyl)carboxamide

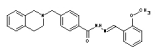
Rotation Bonds: 4

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(F)ccc1)(N\N=C\c1c(c(C)ccc1)O)=O



ID: ST098122

Formula: C25H25N3O2

MW: 399.49

LogP: 5.47

LogS: -5.51

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-methoxyphenyl)-1-azavinyl][4-(2-1,2,3,4-tetrahydroisoquinolylmeth yl)phenyl

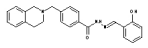
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(CN2Cc3ccccc3CC2)cc1)(N\N=C\c1c(OC)cccc1)=O



ID: ST098123

Formula: C24H23N3O2

MW: 385.47

LogP: 5.06

LogS: -5.2

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl][4-(2-1,2,3,4-tetrahydroisoquinolylmeth yl)phenyl]

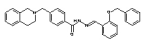
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(CN2Cc3ccccc3CC2)cc1)(N\N=C\c1c(O)cccc1)=O



ID: ST098124

Formula: C31H29N3O2

MW: 475.59

LogP: 7.14

LogS: -6.44

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[2-(phenylmethoxy)phenyl]-1-azavinyl}[4-(2-1,2,3,4-tetrahydroisoquin olylmethy

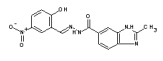
Rotation Bonds: 5

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: C(c1ccc(CN2Cc3ccccc3CC2)cc1)(N\N=C\c1c(OCc2ccccc2)cccc1)=O



ID: ST098125

Formula: C16H13N5O4

MW: 339.31

LogP: 2.39

LogS: -3.9

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-5-nitrophenyl)-1-azavinyl](2-methylbenzimidazol-6-yl)carb oxamide

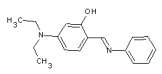
Rotation Bonds: 3

Lipinski: 4

N+O: 9

Chiral Centers: 0

Smiles: [N+](c1cc(/C=N\\NC(c2cc3[nH]c(C)nc3cc2)=O)c(cc1)O)([O-])=O



ID: ST098126

Formula: C17H20N2O

MW: 268.36

LogP: 4.66

LogS: -4.65

Acceptors: 1

Donors: 1

Oil: SOLID

IUPACNAME: 2-((1E)-2-phenyl-2-azavinyl)-5-(diethylamino)phenol

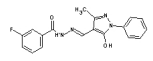
Rotation Bonds: 4

Lipinski: 4

N+O: 3

Chiral Centers: 0

Smiles: c1c(N(CC)CC)ccc(c1O)/C=N\c1ccccc1



ID: ST098127

Formula: C18H15FN4O2

MW: 338.34

LogP: 3.43

LogS: -4.33

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-hydroxy-3-methyl-1-phenylpyrazol-4-yl)-1-azavinyl](3-fluorophenyl)carboxam

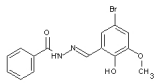
Rotation Bonds: 3

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: n1(c(c(/C=N\NC(c2cc(F)ccc2)=O)c(n1)C)O)c1ccccc1



ID: ST098128

Formula: C15H13BrN2O3

MW: 349.18

LogP: 3.36

LogS: -4.08

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-bromo-2-hydroxy-3-methoxyphenyl)-1-azavinyl]benzamide

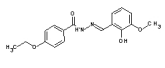
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(c(c(OC)cc(c1)Br)O)/C=N\NC(=O)c1ccccc1



ID: ST098129

Formula: C17H18N2O4

MW: 314.34

LogP: 3.14

LogS: -4.1

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl](4-ethoxyphenyl)carboxamide

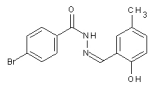
Rotation Bonds: 5

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(c1ccc(cc1)OCC)(N\N=C\c1c(c(OC)ccc1)O)=O



ID: ST098130

Formula: C15H13BrN2O2

MW: 333.18

LogP: 3.94

LogS: -4.26

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1Z)-2-(2-hydroxy-5-methylphenyl)-1-azavinyl](4-bromophenyl)carboxamide

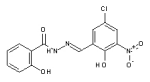
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(c(ccc(c1)C)O)/C=N/NC(c1ccc(cc1)Br)=O



ID: ST098131

Formula: C14H10ClN3O5

MW: 335.7

LogP: 2.94

LogS: -3.91

Acceptors: 5

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-chloro-2-hydroxy-3-nitrophenyl)-1-azavinyl](2-hydroxyphenyl)carbo xamide

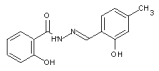
Rotation Bonds: 4

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)c(c(/C=N\NC(c2c(O)cccc2)=O)cc(c1)Cl)O



ID: ST098132

Formula: C15H14N2O3

MW: 270.29

LogP: 2.95

LogS: -3.78

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxy-4-methylphenyl)-1-azavinyl](2-hydroxyphenyl)carboxamide

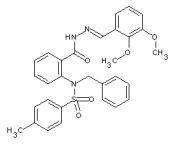
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(N\N=C\c2c(cc(cc2)C)O)=O)c(O)cccc1



ID: ST098133

Formula: C30H29N3O5S

MW: 543.64

LogP: 6.19

LogS: -6.35

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2,3-dimethoxyphenyl)-1-azavinyl](2-{[(4-methylphenyl)sulfonyl]benzy lamino}pl

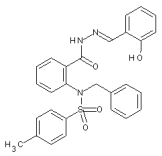
Rotation Bonds: 6

Lipinski: 2

N+O: 8

Chiral Centers: 0

Smiles: S(N(c1c(C(N\N=C\c2c(c(OC)ccc2)OC)=O)cccc1)Cc1ccccc1)(c1ccc(cc1)C)(=O)=O



ID: ST098134

Formula: C28H25N3O4S

MW: 499.59

LogP: 6.02

LogS: -6

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl](2-{[(4-methylphenyl)sulfonyl]benzylami no}pheny

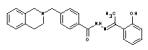
Rotation Bonds: 5

Lipinski: 3

N+O: 7

Chiral Centers: 0

Smiles: S(N(c1c(C(N\N=C\c2c(O)cccc2)=O)cccc1)Cc1ccccc1)(c1ccc(cc1)C)(=O)=O



ID: ST098135

Formula: C25H25N3O2

MW: 399.49

LogP: 5.28

LogS: -5.35

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azaprop-1-enyl][4-(2-1,2,3,4-tetrahydroisoquinol ylmethyl)p

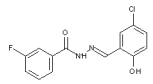
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: N(/NC(c1ccc(CN2Cc3ccccc3CC2)cc1)=O)=C(\c1c(O)cccc1)C



ID: ST098136

Formula: C14H10ClFN2O2

MW: 292.7

LogP: 3.19

LogS: -3.95

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(5-chloro-2-hydroxyphenyl)-1-azavinyl](3-fluorophenyl)carboxamide

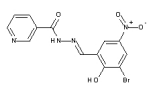
Rotation Bonds: 4

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: C(c1cc(F)ccc1)(N\N=C\c1c(ccc(c1)Cl)O)=O



ID: ST098137

Formula: C13H9BrN4O4

MW: 365.14

LogP: 1.13

LogS: -3.39

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(3-bromo-2-hydroxy-5-nitrophenyl)-1-azavinyl]-3-pyridylcarboxamide

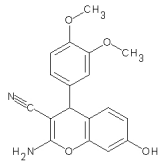
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1cc(Br)c(c(c1)/C=N\NC(c1cnccc1)=O)O)([O-])=O



ID: ST098138

Formula: C18H16N2O4

MW: 324.34

LogP: 2.29

LogS: -3.87

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-4-(3,4-dimethoxyphenyl)-7-hydroxy-4H-chromene-3-carbonitrile

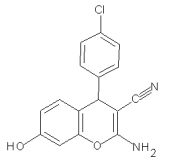
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1cc(OC)c(cc1)OC)ccc(O)c2)N)C#N



ID: ST098139

Formula: C16H11ClN2O2

MW: 298.73

LogP: 3.23

LogS: -4.01

Acceptors: 2

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-4-(4-chlorophenyl)-7-hydroxy-4H-chromene-3-carbonitrile

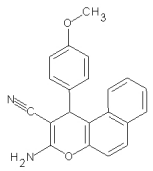
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)Cl)ccc(O)c2)N)C#N



ID: ST098140

Formula: C21H16N2O2

MW: 328.37

LogP: 4.54

LogS: -4.86

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: 3-amino-1-(4-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile

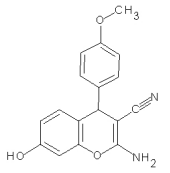
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)OC)c1c(cc2)cccc1)N)C#N



ID: ST098141

Formula: C17H14N2O3

MW: 294.31

LogP: 2.59

LogS: -3.86

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-7-hydroxy-4-(4-methoxyphenyl)-4H-chromene-3-carbonitrile

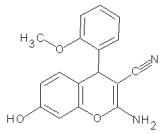
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)OC)ccc(O)c2)N)C#N



ID: ST098142

Formula: C17H14N2O3

MW: 294.31

LogP: 2.71

LogS: -3.89

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-7-hydroxy-4-(2-methoxyphenyl)-4H-chromene-3-carbonitrile

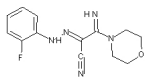
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1c(OC)cccc1)ccc(O)c2)N)C#N



ID: ST098143

Formula: C13H14FN5O

MW: 275.29

LogP: 0.32

LogS: -3.08

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(2-fluorophenyl)amino]-2-(iminomorpholin-4-ylmethyl)-3-azaprop-2-eneni trile

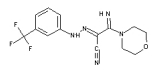
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(F)cccc1)C#N)(N1CCOCC1)=N



ID: ST098144

Formula: C14H14F3N5O

MW: 325.29

LogP: 0.93

LogS: -3.36

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-{[3-(trifluoromethyl)phenyl]amino}-3-azap rop-2-ene

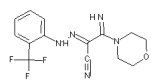
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(C(F)(F)F)ccc1)C#N)(N1CCOCC1)=N



ID: ST098145

Formula: C14H14F3N5O

MW: 325.29

LogP: 0.91

LogS: -3.35

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-{[2-(trifluoromethyl)phenyl]amino}-3-azap rop-2-ene

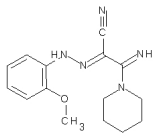
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(C(F)(F)F)cccc1)C#N)(N1CCOCC1)=N



ID: ST098146

Formula: C15H19N5O

MW: 285.35

LogP: 1.96

LogS: -3.7

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminopiperidylmethyl)-3-[(2-methoxyphenyl)amino]-3-azaprop-2-enenitril e

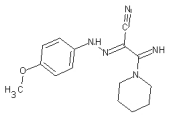
Rotation Bonds: 2

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(OC)cccc1)C#N)(N1CCCCC1)=N



ID: ST098147

Formula: C15H19N5O

MW: 285.35

LogP: 1.95

LogS: -3.71

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminopiperidylmethyl)-3-[(4-methoxyphenyl)amino]-3-azaprop-2-enenitril e

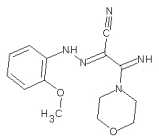
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)OC)C#N)(N1CCCCC1)=N



ID: ST098148

Formula: C14H17N5O2

MW: 287.32

LogP: 0.25

LogS: -3.17

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-[(2-methoxyphenyl)amino]-3-azaprop-2-enen itrile

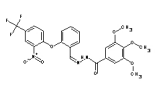
Rotation Bonds: 2

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(/C(=N\Nc1c(OC)cccc1)C#N)(N1CCOCC1)=N



ID: ST098149

Formula: C24H20F3N3O7

MW: 519.43

LogP: 4.62

LogS: -5.33

Acceptors: 7

Donors: 1

Oil: SOLID

IUPACNAME: N-((1Z)-2-{2-[2-nitro-4-(trifluoromethyl)phenoxy]phenyl}-1-azavinyl)(3,4,5-tri methoxyphen

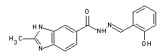
Rotation Bonds: 5

Lipinski: 3

N+O: 10

Chiral Centers: 0

Smiles: c1([N+]([O-])=O)c(Oc2c(/C=N/NC(c3cc(OC)c(c(c3)OC)OC)=O)cccc2)ccc(C(F)(F)F)c1



ID: ST098150

Formula: C16H14N4O2

MW: 294.31

LogP: 2.74

LogS: -3.91

Acceptors: 2

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl](2-methylbenzimidazol-6-yl)carboxamide

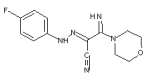
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: n1c([nH]c2c1ccc(C(N\N=C\c1c(O)cccc1)=O)c2)C



ID: ST098151

Formula: C13H14FN5O

MW: 275.29

LogP: 0.4

LogS: -3.12

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(4-fluorophenyl)amino]-2-(iminomorpholin-4-ylmethyl)-3-azaprop-2-eneni trile

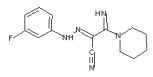
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)F)C#N)(N1CCOCC1)=N



ID: ST098152

Formula: C14H16FN5

MW: 273.31

LogP: 2.09

LogS: -3.65

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(3-fluorophenyl)amino]-2-(iminopiperidylmethyl)-3-azaprop-2-enenitrile

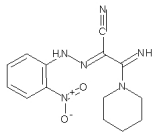
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(F)ccc1)C#N)(N1CCCCC1)=N



ID: ST098153

Formula: C14H16N6O2

MW: 300.32

LogP: 1.89

LogS: -3.67

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminopiperidylmethyl)-3-[(2-nitrophenyl)amino]-3-azaprop-2-enenitrile

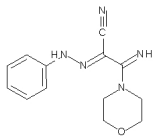
Rotation Bonds: 2

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1c(N\N=C(\C(N2CCCCC2)=N)C#N)cccc1)([O-])=O



ID: ST098154

Formula: C13H15N5O

MW: 257.3

LogP: 0.44

LogS: -3.11

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-(phenylamino)-3-azaprop-2-enenitrile

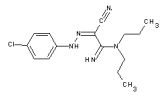
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccccc1)C#N)(N1CCOCC1)=N



ID: ST098155

Formula: C15H20ClN5

MW: 305.81

LogP: 3.33

LogS: -4.21

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2Z)-2-[(dipropylamino)iminomethyl]-3-[(4-chlorophenyl)amino]-3-azaprop-2-enen itrile

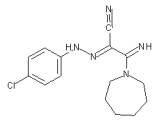
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N)N(CCC)CCC)(=N/Nc1ccc(cc1)Cl)C#N



ID: ST098156

Formula: C15H18ClN5

MW: 303.79

LogP: 3.12

LogS: -4.11

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(azaperhydroepinyliminomethyl)-3-[(4-chlorophenyl)amino]-3-azaprop-2-en enitrile

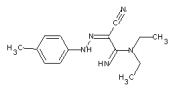
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)Cl)C#N)(N1CCCCCC1)=N



ID: ST098157

Formula: C14H19N5

MW: 257.34

LogP: 2.34

LogS: -3.75

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2Z)-2-[(diethylamino)iminomethyl]-3-[(4-methylphenyl)amino]-3-azaprop-2-eneni trile

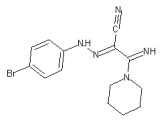
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N)N(CC)CC)(=N/Nc1ccc(cc1)C)C#N



ID: ST098158

Formula: C14H16BrN5

MW: 334.22

LogP: 2.76

LogS: -3.95

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(4-bromophenyl)amino]-2-(iminopiperidylmethyl)-3-azaprop-2-enenitrile

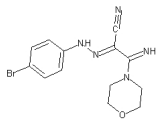
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)Br)C#N)(N1CCCCC1)=N



ID: ST098159

Formula: C13H14BrN5O

MW: 336.19

LogP: 1.06

LogS: -3.41

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(4-bromophenyl)amino]-2-(iminomorpholin-4-ylmethyl)-3-azaprop-2-enenit rile

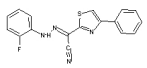
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)Br)C#N)(N1CCOCC1)=N



ID: ST098160

Formula: C17H11FN4S

MW: 322.37

LogP: 3.9

LogS: -4.48

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-3-[(2-fluorophenyl)amino]-2-(4-phenyl(1,3-thiazol-2-yl))-3-azaprop-2-enen itrile

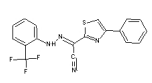
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2c(F)cccc2)C#N)scc1c1ccccc1



ID: ST098161

Formula: C18H11F3N4S

MW: 372.37

LogP: 4.5

LogS: -4.75

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-(4-phenyl(1,3-thiazol-2-yl))-3-{[2-(trifluoromethyl)phenyl]amino}-3-aza prop-2-enen

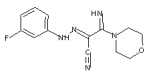
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2c(C(F)(F)F)cccc2)C#N)scc1c1ccccc1



ID: ST098162

Formula: C13H14FN5O

MW: 275.29

LogP: 0.38

LogS: -3.11

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-3-[(3-fluorophenyl)amino]-2-(iminomorpholin-4-ylmethyl)-3-azaprop-2-eneni trile

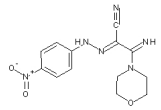
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(F)ccc1)C#N)(N1CCOCC1)=N



ID: ST098163

Formula: C13H14N6O3

MW: 302.29

LogP: -0.06

LogS: -3.06

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-[(4-nitrophenyl)amino]-3-azaprop-2-enenit rile

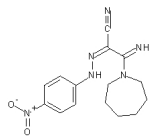
Rotation Bonds: 2

Lipinski: 4

N+O: 9

Chiral Centers: 0

Smiles: [N+](c1ccc(N\N=C(\C(N2CCOCC2)=N)C#N)cc1)([O-])=O



ID: ST098164

Formula: C15H18N6O2

MW: 314.35

LogP: 2.15

LogS: -3.83

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2Z)-2-(azaperhydroepinyliminomethyl)-3-[(4-nitrophenyl)amino]-3-azaprop-2-ene nitrile

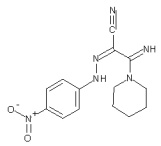
Rotation Bonds: 2

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1ccc(N\N=C(/C(N2CCCCCC2)=N)C#N)cc1)([O-])=O



ID: ST098165

Formula: C14H16N6O2

MW: 300.32

LogP: 1.65

LogS: -3.6

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2Z)-2-(iminopiperidylmethyl)-3-[(4-nitrophenyl)amino]-3-azaprop-2-enenitrile

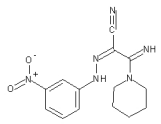
Rotation Bonds: 2

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1ccc(N\N=C(/C(N2CCCCC2)=N)C#N)cc1)([O-])=O



ID: ST098166

Formula: C14H16N6O2

MW: 300.32

LogP: 1.83

LogS: -3.65

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2Z)-2-(iminopiperidylmethyl)-3-[(3-nitrophenyl)amino]-3-azaprop-2-enenitrile

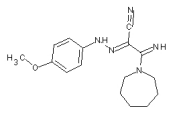
Rotation Bonds: 2

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: [N+](c1cc(N\N=C(/C(N2CCCCC2)=N)C#N)ccc1)([O-])=O



ID: ST098167

Formula: C16H21N5O

MW: 299.38

LogP: 2.45

LogS: -3.94

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(azaperhydroepinyliminomethyl)-3-[(4-methoxyphenyl)amino]-3-azaprop-2-e nenitr

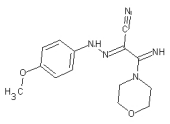
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)OC)C#N)(N1CCCCCC1)=N



ID: ST098168

Formula: C14H17N5O2

MW: 287.32

LogP: 0.25

LogS: -3.17

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(iminomorpholin-4-ylmethyl)-3-[(4-methoxyphenyl)amino]-3-azaprop-2-enen itrile

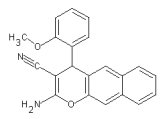
Rotation Bonds: 1

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)OC)C#N)(N1CCOCC1)=N



ID: ST098169

Formula: C21H16N2O2

MW: 328.37

LogP: 4.63

LogS: -4.89

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(2-methoxyphenyl)-4H-benzo[g]chromene-3-carbonitrile

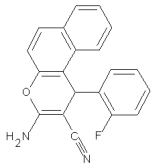
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C=1(C(c2cc3ccccc3cc2OC1N)c1c(OC)cccc1)C#N



ID: ST098170

Formula: C20H13FN2O

MW: 316.33

LogP: 4.72

LogS: -4.81

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 3-amino-1-(2-fluorophenyl)-1H-benzo[f]chromene-2-carbonitrile

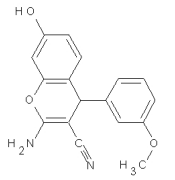
Rotation Bonds: 1

Lipinski: 4

N+O: 3

Chiral Centers: 1

Smiles: C=1(C(c2c3c(cccc3)ccc2OC1N)c1c(F)cccc1)C#N



ID: ST098171

Formula: C17H14N2O3

MW: 294.31

LogP: 2.59

LogS: -3.85

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-7-hydroxy-4-(3-methoxyphenyl)-4H-chromene-3-carbonitrile

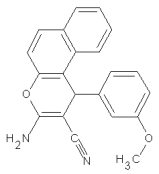
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1cc(OC)ccc1)ccc(O)c2)N)C#N



ID: ST098172

Formula: C21H16N2O2

MW: 328.37

LogP: 4.54

LogS: -4.86

Acceptors: 2

Donors: 2

Oil: SOLID

IUPACNAME: 3-amino-1-(3-methoxyphenyl)-1H-benzo[f]chromene-2-carbonitrile

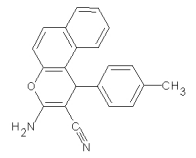
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C=1(C(c2c3c(cccc3)ccc2OC1N)c1cc(OC)ccc1)C#N



ID: ST098173

Formula: C21H16N2O

MW: 312.37

LogP: 5.03

LogS: -4.97

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 3-amino-1-(4-methylphenyl)-1H-benzo[f]chromene-2-carbonitrile

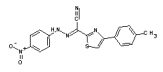
Rotation Bonds: 0

Lipinski: 4

N+O: 3

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)C)c1c(cc2)cccc1)N)C#N



ID: ST098174

Formula: C18H13N5O2S

MW: 363.4

LogP: 3.93

LogS: -4.66

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-methylphenyl)(1,3-thiazol-2-yl)]-3-[(4-nitrophenyl)amino]-3-azapr op-2-enenitr

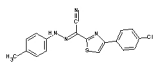
Rotation Bonds: 1

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc([N+]([O-])=O)cc2)C#N)scc1c1ccc(cc1)C



ID: ST098175

Formula: C18H13ClN4S

MW: 352.85

LogP: 4.86

LogS: -4.93

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-chlorophenyl)(1,3-thiazol-2-yl)]-3-[(4-methylphenyl)amino]-3-azap rop-2-ener

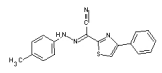
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)C)C#N)scc1c1ccc(cc1)Cl



ID: ST098176

Formula: C18H14N4S

MW: 318.4

LogP: 4.51

LogS: -4.74

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-3-[(4-methylphenyl)amino]-2-(4-phenyl(1,3-thiazol-2-yl))-3-azaprop-2-enen itrile

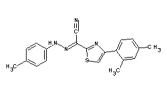
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)C)C#N)scc1c1ccccc1



ID: ST098177

Formula: C20H18N4S

MW: 346.46

LogP: 5.33

LogS: -5.15

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(2,4-dimethylphenyl)(1,3-thiazol-2-yl)]-3-[(4-methylphenyl)amino]-3- azaprop-2-e

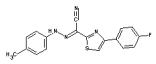
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)C)C#N)scc1c1c(cc(cc1)C)C



ID: ST098178

Formula: C18H13FN4S

MW: 336.39

LogP: 4.34

LogS: -4.7

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-fluorophenyl)(1,3-thiazol-2-yl)]-3-[(4-methylphenyl)amino]-3-azap rop-2-enen

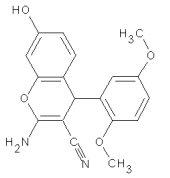
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)C)C#N)scc1c1ccc(cc1)F



ID: ST098179

Formula: C18H16N2O4

MW: 324.34

LogP: 2.52

LogS: -3.95

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-4-(2,5-dimethoxyphenyl)-7-hydroxy-4H-chromene-3-carbonitrile

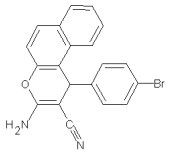
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 1

Smiles: C=1(C(c2c(ccc(c2)OC)OC)c2ccc(cc2OC1N)O)C#N



ID: ST098180

Formula: C20H13BrN2O

MW: 377.24

LogP: 5.36

LogS: -5.1

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 3-amino-1-(4-bromophenyl)-1H-benzo[f]chromene-2-carbonitrile

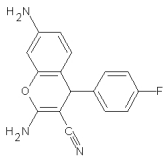
Rotation Bonds: 0

Lipinski: 4

N+O: 3

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)Br)c1c(cc2)cccc1)N)C#N



ID: ST098181

Formula: C16H12FN3O

MW: 281.29

LogP: 2.56

LogS: -3.83

Acceptors: 1

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(4-fluorophenyl)-4H-chromene-3-carbonitrile

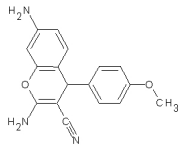
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)F)ccc(N)c2)N)C#N



ID: ST098182

Formula: C17H15N3O2

MW: 293.33

LogP: 2.44

LogS: -3.9

Acceptors: 2

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(4-methoxyphenyl)-4H-chromene-3-carbonitrile

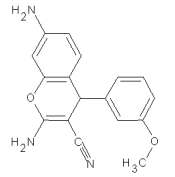
Rotation Bonds: 0

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc(cc1)OC)ccc(N)c2)N)C#N



ID: ST098183

Formula: C17H15N3O2

MW: 293.33

LogP: 2.44

LogS: -3.9

Acceptors: 2

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(3-methoxyphenyl)-4H-chromene-3-carbonitrile

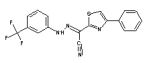
Rotation Bonds: 2

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1cc(OC)ccc1)ccc(N)c2)N)C#N



ID: ST098184

Formula: C18H11F3N4S

MW: 372.37

LogP: 4.52

LogS: -4.76

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-(4-phenyl(1,3-thiazol-2-yl))-3-{[3-(trifluoromethyl)phenyl]amino}-3-aza prop-2-enen

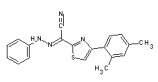
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2cc(C(F)(F)F)ccc2)C#N)scc1c1ccccc1



ID: ST098185

Formula: C19H16N4S

MW: 332.43

LogP: 4.85

LogS: -4.92

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(2,4-dimethylphenyl)(1,3-thiazol-2-yl)]-3-(phenylamino)-3-azaprop-2- enenitrile

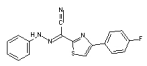
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccccc2)C#N)scc1c1c(cc(cc1)C)C



ID: ST098186

Formula: C17H11FN4S

MW: 322.37

LogP: 3.86

LogS: -4.48

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-fluorophenyl)(1,3-thiazol-2-yl)]-3-(phenylamino)-3-azaprop-2-enen itrile

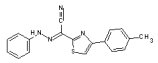
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccccc2)C#N)scc1c1ccc(cc1)F



ID: ST098187

Formula: C18H14N4S

MW: 318.4

LogP: 4.43

LogS: -4.72

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-methylphenyl)(1,3-thiazol-2-yl)]-3-(phenylamino)-3-azaprop-2-enen itrile

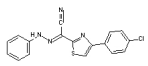
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccccc2)C#N)scc1c1ccc(cc1)C



ID: ST098188

Formula: C17H11ClN4S

MW: 338.82

LogP: 4.38

LogS: -4.7

Acceptors: 0

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-chlorophenyl)(1,3-thiazol-2-yl)]-3-(phenylamino)-3-azaprop-2-enen itrile

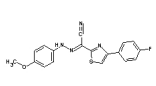
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccccc2)C#N)scc1c1ccc(cc1)Cl



ID: ST098189

Formula: C18H13FN4OS

MW: 352.39

LogP: 3.66

LogS: -4.53

Acceptors: 1

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-fluorophenyl)(1,3-thiazol-2-yl)]-3-[(4-methoxyphenyl)amino]-3-aza prop-2-ene

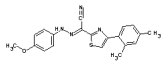
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)OC)C#N)scc1c1ccc(cc1)F



ID: ST098190

Formula: C20H18N4OS

MW: 362.46

LogP: 4.65

LogS: -4.98

Acceptors: 1

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(2,4-dimethylphenyl)(1,3-thiazol-2-yl)]-3-[(4-methoxyphenyl)amino]-3 -azaprop-2

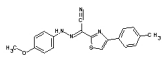
Rotation Bonds: 2

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)OC)C#N)scc1c1c(cc(cc1)C)C



ID: ST098191

Formula: C19H16N4OS

MW: 348.43

LogP: 4.24

LogS: -4.78

Acceptors: 1

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-3-[(4-methoxyphenyl)amino]-2-[4-(4-methylphenyl)(1,3-thiazol-2-yl)]-3-aza prop-2-en

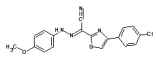
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)OC)C#N)scc1c1ccc(cc1)C



ID: ST098192

Formula: C18H13ClN4OS

MW: 368.85

LogP: 4.18

LogS: -4.76

Acceptors: 1

Donors: 1

Oil: SOLID

IUPACNAME: (2E)-2-[4-(4-chlorophenyl)(1,3-thiazol-2-yl)]-3-[(4-methoxyphenyl)amino]-3-aza prop-2-en

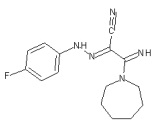
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: n1c(/C(=N\Nc2ccc(cc2)OC)C#N)scc1c1ccc(cc1)Cl



ID: ST098193

Formula: C15H18FN5

MW: 287.34

LogP: 2.61

LogS: -3.89

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(azaperhydroepinyliminomethyl)-3-[(4-fluorophenyl)amino]-3-azaprop-2-en enitrile

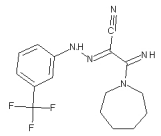
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1ccc(cc1)F)C#N)(N1CCCCCC1)=N



ID: ST098194

Formula: C16H18F3N5

MW: 337.35

LogP: 3.14

LogS: -4.13

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(azaperhydroepinyliminomethyl)-3-{[3-(trifluoromethyl)phenyl]amino}-3-a zaprop-2-

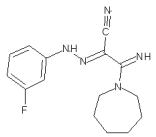
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(C(F)(F)F)ccc1)C#N)(N1CCCCCC1)=N



ID: ST098195

Formula: C15H18FN5

MW: 287.34

LogP: 2.59

LogS: -3.88

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: (2E)-2-(azaperhydroepinyliminomethyl)-3-[(3-fluorophenyl)amino]-3-azaprop-2-en enitrile

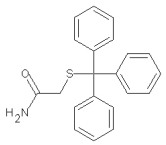
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: C(/C(=N\Nc1cc(F)ccc1)C#N)(N1CCCCCC1)=N



ID: ST098196

Formula: C21H19NOS

MW: 333.45

LogP: 6.2

LogS: -5.34

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-(triphenylmethylthio)acetamide

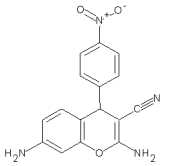
Rotation Bonds: 2

Lipinski: 3

N+O: 2

Chiral Centers: 0

Smiles: C(SCC(=O)N)(c1ccccc1)(c1ccccc1)c1ccccc1



ID: ST098197

Formula: C16H12N4O3

MW: 308.3

LogP: 2.28

LogS: -3.83

Acceptors: 3

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(4-nitrophenyl)-4H-chromene-3-carbonitrile

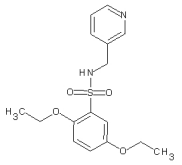
Rotation Bonds: 0

Lipinski: 4

N+O: 7

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1ccc([N+]([O-])=O)cc1)ccc(N)c2)N)C#N



ID: ST098198

Formula: C16H20N2O4S

MW: 336.41

LogP: 2.44

LogS: -4.19

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: [(2,5-diethoxyphenyl)sulfonyl](3-pyridylmethyl)amine

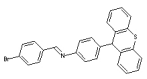
Rotation Bonds: 7

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: S(c1cc(OCC)ccc1OCC)(NCc1cnccc1)(=O)=O



ID: ST098199

Formula: C26H18BrNS

MW: 456.41

LogP: 9.83

LogS: -6.97

Acceptors: 0

Donors: 0

Oil: SOLID

IUPACNAME: 10-{4-[(1E)-2-(4-bromophenyl)-1-azavinyl]phenyl}-10H-dibenzo[b,e]thiin

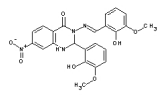
Rotation Bonds: 0

Lipinski: 3

N+O: 1

Chiral Centers: 0

Smiles: S1c2c(cccc2)C(c2c1cccc2)c1ccc(/N=C\c2ccc(cc2)Br)cc1



ID: ST098200

Formula: C23H20N4O7

MW: 464.43

LogP: 2.46

LogS: -4.38

Acceptors: 7

Donors: 3

Oil: SOLID

IUPACNAME: 3-[(1E)-2-(2-hydroxy-3-methoxyphenyl)-1-azavinyl]-2-(2-hydroxy-3-methoxyphenyl)-7-nitr

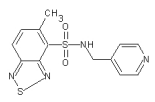
Rotation Bonds: 7

Lipinski: 4

N+O: 11

Chiral Centers: 1

Smiles: N1(C(Nc2c(C1=O)ccc([N+]([O-])=O)c2)c1c(c(OC)ccc1)O)\N=C\c1c(c(OC)ccc1)O



ID: ST098201

Formula: C13H12N4O2S2

MW: 320.4

LogP: 1.59

LogS: -3.86

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: [(5-methylbenzo[c]1,2,5-thiadiazol-4-yl)sulfonyl](4-pyridylmethyl)amine

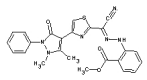
Rotation Bonds: 2

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: c1(S(NCc2ccnc2)(=O)=O)c2c(nsn2)ccc1C



ID: ST098202

Formula: C24H20N6O3S

MW: 472.53

LogP: 3.98

LogS: -5.26

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: methyl 2-({(1E)-2-[4-(2,3-dimethyl-5-oxo-1-phenyl(3-pyrazolin-4-yl))(1,3-thiaz ol-2-yl)]-2-cy

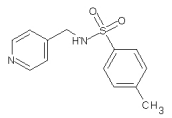
Rotation Bonds: 4

Lipinski: 4

N+O: 9

Chiral Centers: 0

Smiles: c1(c(n(c2ccccc2)n(c1C)C)=O)c1nc(/C(=N\Nc2c(C(=O)OC)cccc2)C#N)sc1



ID: ST098203

Formula: C13H14N2O2S

MW: 262.33

LogP: 2.11

LogS: -3.78

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: [(4-methylphenyl)sulfonyl](4-pyridylmethyl)amine

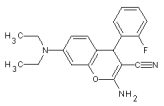
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: S(NCc1ccncc1)(c1ccc(cc1)C)(=O)=O



ID: ST098204

Formula: C20H20FN3O

MW: 337.4

LogP: 4.62

LogS: -4.87

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(diethylamino)-4-(2-fluorophenyl)-4H-chromene-3-carbonitrile

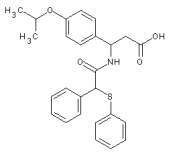
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: C1(=C(Oc2c(C1c1c(F)cccc1)ccc(N(CC)CC)c2)N)C#N



ID: ST098205

Formula: C26H27NO4S

MW: 449.57

LogP: 6.98

LogS: -6.03

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: 3-[4-(methylethoxy)phenyl]-3-(2-phenyl-2-phenylthioacetylamino)propanoic acid

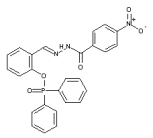
Rotation Bonds: 7

Lipinski: 3

N+O: 5

Chiral Centers: 2

Smiles: C(NC(CC(=O)O)c1ccc(OC(C)C)cc1)(C(Sc1ccccc1)c1ccccc1)=O



ID: ST098206

Formula: C26H20N3O5P

MW: 485.44

LogP: 4.61

LogS: -5.48

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-{(1E)-2-[2-(diphenylcarbonyloxy)phenyl]-1-azavinyl}(4-nitrophenyl)carboxamid e

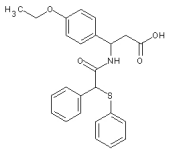
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: P(Oc1c(/C=N\NC(c2ccc([N+]([O-])=O)cc2)=O)cccc1)(=O)(c1ccccc1)c1ccccc1



ID: ST098207

Formula: C25H25NO4S

MW: 435.54

LogP: 6.42

LogS: -5.78

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: 3-(4-ethoxyphenyl)-3-(2-phenyl-2-phenylthioacetylamino)propanoic acid

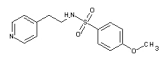
Rotation Bonds: 7

Lipinski: 3

N+O: 5

Chiral Centers: 2

Smiles: C(NC(CC(=O)O)c1ccc(cc1)OCC)(C(Sc1ccccc1)c1ccccc1)=O



ID: ST098208

Formula: C14H16N2O3S

MW: 292.36

LogP: 2.13

LogS: -3.89

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-methoxyphenyl)sulfonyl](2-(4-pyridyl)ethyl)amine

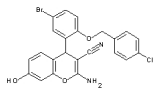
Rotation Bonds: 2

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1ccc(cc1)OC)(=O)(=O)NCCc1ccncc1



ID: ST098209

Formula: C23H16BrClN2O3

MW: 483.75

LogP: 5.66

LogS: -5.39

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: 2-amino-4-{5-bromo-2-[(4-chlorophenyl)methoxy]phenyl}-7-hydroxy-4H-chromene-3- carb

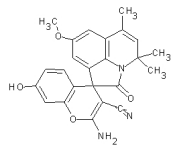
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C=1(C(c2c(OCc3ccc(cc3)Cl)ccc(c2)Br)c2ccc(cc2OC1N)O)C#N



ID: ST098210

Formula: C24H21N3O4

MW: 415.45

LogP: 3.75

LogS: -4.8

Acceptors: 4

Donors: 3

Oil: SOLID

IUPACNAME:

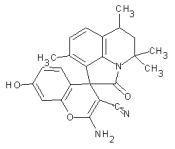
Rotation Bonds: 2

Lipinski: 4

N+O: 7

Chiral Centers: 1

Smiles: N12C(C3(C(=C(N)Oc4c3ccc(O)c4)C#N)c3c2c(C(C)=CC1(C)C)cc(c3)OC)=O



ID: ST098211

Formula: C24H23N3O3

MW: 401.47

LogP: 4.53

LogS: -5.01

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME:

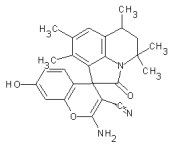
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 2

Smiles: N12C(C3(C(=C(N)Oc4c3ccc(O)c4)C#N)c3c2c(C(C)CC1(C)C)ccc3C)=O



ID: ST098212

Formula: C25H25N3O3

MW: 415.49

LogP: 4.97

LogS: -5.23

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME:

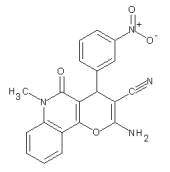
Rotation Bonds: 1

Lipinski: 4

N+O: 6

Chiral Centers: 2

Smiles: N12C(C3(C(=C(N)Oc4c3ccc(O)c4)C#N)c3c2c(C(C)CC1(C)C)cc(c3C)C)=O



ID: ST098213

Formula: C20H14N4O4

MW: 374.36

LogP: 3.47

LogS: -4.59

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-6-methyl-4-(3-nitrophenyl)-5-oxo-6-hydro-4H-pyrano[3,2-c]quinoline-3-c arbonitri

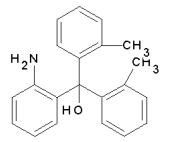
Rotation Bonds: 1

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: c12c(OC(N)=C(C2c2cc([N+]([O-])=O)ccc2)C#N)c2ccccc2n(c1=O)C



ID: ST098214

Formula: C21H21NO

MW: 303.4

LogP: 6.11

LogS: -5.29

Acceptors: 1

Donors: 3

Oil: SOLID

IUPACNAME: (2-aminophenyl)bis(2-methylphenyl)methan-1-ol

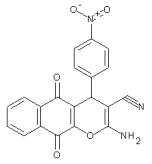
Rotation Bonds: 4

Lipinski: 3

N+O: 2

Chiral Centers: 0

Smiles: C(c1c(N)cccc1)(c1c(C)cccc1)(c1c(C)cccc1)O



ID: ST098215

Formula: C20H11N3O5

MW: 373.32

LogP: 1.58

LogS: -3.96

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(4-nitrophenyl)-5,10-dioxo-4H-benzo[g]chromene-3-carbonitrile

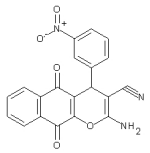
Rotation Bonds: 0

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: C1(c2c(cccc2)C(C2=C1OC(=C(C2c1ccc(cc1)[N+]([O-])=O)C#N)N)=O)=O



ID: ST098216

Formula: C20H11N3O5

MW: 373.32

LogP: 1.56

LogS: -3.95

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(3-nitrophenyl)-5,10-dioxo-4H-benzo[g]chromene-3-carbonitrile

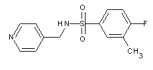
Rotation Bonds: 1

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: C1(c2c(cccc2)C(C2=C1OC(=C(C2c1cccc(c1)[N+]([O-])=O)C#N)N)=O)=O



ID: ST098217

Formula: C13H13FN2O2S

MW: 280.32

LogP: 2.05

LogS: -3.77

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: [(4-fluoro-3-methylphenyl)sulfonyl](4-pyridylmethyl)amine

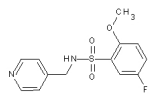
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: N(Cc1ccncc1)S(c1cc(c(F)cc1)C)(=O)=O



ID: ST098218

Formula: C13H13FN2O3S

MW: 296.32

LogP: 1.38

LogS: -3.61

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(5-fluoro-2-methoxyphenyl)sulfonyl](4-pyridylmethyl)amine

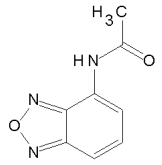
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: N(Cc1ccncc1)S(c1cc(ccc1OC)F)(=O)=O



ID: ST098219

Formula: C8H7N3O2

MW: 177.16

LogP: 0.69

LogS: -2.84

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-benzo[2,3-c]1,2,5-oxadiazol-4-ylacetamide

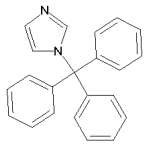
Rotation Bonds: 0

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c12cccc(c1non2)NC(C)=O



ID: ST098220

Formula: C22H18N2

MW: 310.4

LogP: 6.09

LogS: -5.45

Acceptors: 0

Donors: 0

Oil: SOLID

IUPACNAME: (triphenylmethyl)imidazole

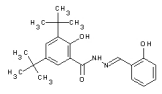
Rotation Bonds: 0

Lipinski: 3

N+O: 2

Chiral Centers: 0

Smiles: c1cncn1C(c1ccccc1)(c1ccccc1)c1ccccc1



ID: ST098221

Formula: C22H28N2O3

MW: 368.48

LogP: 6.09

LogS: -5.34

Acceptors: 3

Donors: 3

Oil: SOLID

IUPACNAME: N-[(1E)-2-(2-hydroxyphenyl)-1-azavinyl][3,5-bis(tert-butyl)-2-hydroxyphenyl]ca rboxamide

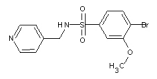
Rotation Bonds: 5

Lipinski: 3

N+O: 5

Chiral Centers: 0

Smiles: c1(c(c(cc(c1)C(C)(C)C)C(C)(C)C)O)C(N\N=C\c1c(O)cccc1)=O



ID: ST098222

Formula: C13H13BrN2O3S

MW: 357.23

LogP: 2.07

LogS: -3.91

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-bromo-3-methoxyphenyl)sulfonyl](4-pyridylmethyl)amine

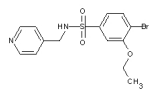
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(OC)c(cc1)Br)(NCc1ccncc1)(=O)=O



ID: ST098223

Formula: C14H15BrN2O3S

MW: 371.25

LogP: 2.6

LogS: -4.15

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-bromo-3-ethoxyphenyl)sulfonyl](4-pyridylmethyl)amine

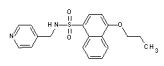
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(OCC)c(cc1)Br)(NCc1ccncc1)(=O)=O



ID: ST098224

Formula: C19H20N2O3S

MW: 356.45

LogP: 3.98

LogS: -4.85

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-propoxynaphthyl)sulfonyl](4-pyridylmethyl)amine

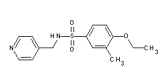
Rotation Bonds: 5

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1c2c(cccc2)c(cc1)OCCC)(NCc1ccncc1)(=O)=O



ID: ST098225

Formula: C15H18N2O3S

MW: 306.39

LogP: 2.55

LogS: -4.1

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-ethoxy-3-methylphenyl)sulfonyl](4-pyridylmethyl)amine

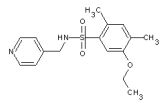
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(C)c(cc1)OCC)(NCc1ccncc1)(=O)=O



ID: ST098226

Formula: C16H20N2O3S

MW: 320.41

LogP: 3.04

LogS: -4.34

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(5-ethoxy-2,4-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

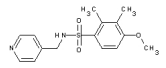
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(OCC)c(cc1C)C)(NCc1ccncc1)(=O)=O



ID: ST098227

Formula: C15H18N2O3S

MW: 306.39

LogP: 2.43

LogS: -4.07

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-methoxy-2,3-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

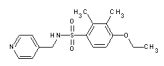
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1c(c(C)c(cc1)OC)C)(NCc1ccncc1)(=O)=O



ID: ST098228

Formula: C16H20N2O3S

MW: 320.41

LogP: 3.01

LogS: -4.32

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-ethoxy-2,3-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

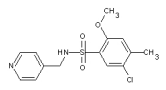
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1c(c(C)c(cc1)OCC)C)(NCc1ccncc1)(=O)=O



ID: ST098229

Formula: C14H15ClN2O3S

MW: 326.8

LogP: 2.38

LogS: -4.06

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(5-chloro-2-methoxy-4-methylphenyl)sulfonyl](4-pyridylmethyl)amine

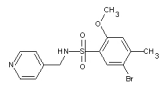
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(Cl)c(cc1OC)C)(NCc1ccncc1)(=O)=O



ID: ST098230

Formula: C14H15BrN2O3S

MW: 371.25

LogP: 2.49

LogS: -4.12

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(5-bromo-2-methoxy-4-methylphenyl)sulfonyl](4-pyridylmethyl)amine

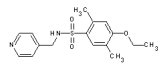
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(Br)c(cc1OC)C)(NCc1ccncc1)(=O)=O



ID: ST098231

Formula: C16H20N2O3S

MW: 320.41

LogP: 3.04

LogS: -4.33

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(4-ethoxy-2,5-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

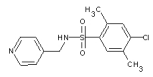
Rotation Bonds: 4

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(C)c(cc1C)OCC)(NCc1ccncc1)(=O)=O



ID: ST098232

Formula: C14H15ClN2O2S

MW: 310.8

LogP: 3.04

LogS: -4.22

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: [(4-chloro-2,5-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

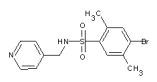
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: S(c1cc(C)c(cc1C)Cl)(NCc1ccncc1)(=O)=O



ID: ST098233

Formula: C14H15BrN2O2S

MW: 355.26

LogP: 3.21

LogS: -4.3

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: [(4-bromo-2,5-dimethylphenyl)sulfonyl](4-pyridylmethyl)amine

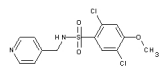
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: S(c1cc(C)c(cc1C)Br)(NCc1ccncc1)(=O)=O



ID: ST098234

Formula: C13H12Cl2N2O3S

MW: 347.22

LogP: 2.36

LogS: -4.04

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: [(2,5-dichloro-4-methoxyphenyl)sulfonyl](4-pyridylmethyl)amine

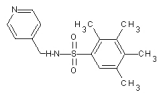
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: S(c1cc(Cl)c(cc1Cl)OC)(NCc1ccncc1)(=O)=O



ID: ST098235

Formula: C16H20N2O2S

MW: 304.41

LogP: 3.43

LogS: -4.42

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: (4-pyridylmethyl)[(2,3,4,5-tetramethylphenyl)sulfonyl]amine

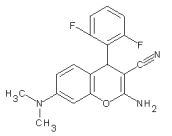
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: S(c1c(c(C)c(c(c1)C)C)C)(NCc1ccncc1)(=O)=O



ID: ST098236

Formula: C18H15F2N3O

MW: 327.33

LogP: 3.64

LogS: -4.43

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(2,6-difluorophenyl)-7-(dimethylamino)-4H-chromene-3-carbonitrile

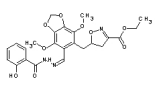
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(C(C(=C(O1)N)C#N)c1c(cccc1F)F)ccc(c2)N(C)C



ID: ST098237

Formula: C24H25N3O9

MW: 499.48

LogP: 2.75

LogS: -4.69

Acceptors: 9

Donors: 2

Oil: SOLID

IUPACNAME: ethyl 5-[(6-{(1Z)-2-[(2-hydroxyphenyl)carbonylamino]-2-azavinyl}-4,7-dimethoxy -2H-benz

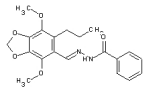
Rotation Bonds: 10

Lipinski: 4

N+O: 12

Chiral Centers: 1

Smiles: c1(c(c(c2c(c1OC)OCO2)OC)CC1ON=C(C1)C(=O)OCC)/C=N/NC(=O)c1c(cccc1)O



ID: ST098238

Formula: C20H22N2O5

MW: 370.41

LogP: 3.53

LogS: -4.58

Acceptors: 5

Donors: 1

Oil: SOLID

IUPACNAME: N-[(1E)-2-(4,7-dimethoxy-6-propyl(2H-benzo[d]1,3-dioxolan-5-yl))-1-azavinyl]be nzamide

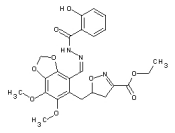
Rotation Bonds: 5

Lipinski: 4

N+O: 7

Chiral Centers: 0

Smiles: c1(c(c(c2c(c1OC)OCO2)OC)CCC)/C=N\NC(=O)c1ccccc1



ID: ST098239

Formula: C24H25N3O9

MW: 499.48

LogP: 2.8

LogS: -4.7

Acceptors: 9

Donors: 2

Oil: SOLID

IUPACNAME: ethyl 5-[(4-{(1Z)-2-[(2-hydroxyphenyl)carbonylamino]-2-azavinyl}-6,7-dimethoxy -2H-benz

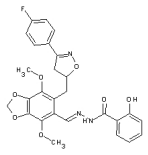
Rotation Bonds: 10

Lipinski: 4

N+O: 12

Chiral Centers: 1

Smiles: c1(c(c(c2c(c1OC)OCO2)/C=N/NC(=O)c1ccccc1O)CC1ON=C(C1)C(=O)OCC)OC



ID: ST098240

Formula: C27H24FN3O7

MW: 521.5

LogP: 4.52

LogS: -5.36

Acceptors: 7

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(6-{[3-(4-fluorophenyl)(4,5-dihydroisoxazol-5-yl)]methyl}-4,7-dimeth oxy(2H-ben

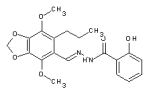
Rotation Bonds: 7

Lipinski: 3

N+O: 10

Chiral Centers: 1

Smiles: c12c(c(OC)c(c(c1OC)CC1ON=C(C1)c1ccc(cc1)F)/C=N\NC(c1c(O)cccc1)=O)OCO2



ID: ST098241

Formula: C20H22N2O6

MW: 386.4

LogP: 3.18

LogS: -4.41

Acceptors: 6

Donors: 2

Oil: SOLID

IUPACNAME: N-[(1E)-2-(4,7-dimethoxy-6-propyl(2H-benzo[3,4-d]1,3-dioxolen-5-yl))-1-azaviny l](2-hydr

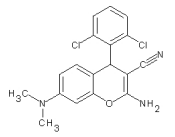
Rotation Bonds: 7

Lipinski: 4

N+O: 8

Chiral Centers: 0

Smiles: c12c(c(c(CCC)c(c1OC)/C=N\NC(c1c(O)cccc1)=O)OC)OCO2



ID: ST098242

Formula: C18H15Cl2N3O

MW: 360.24

LogP: 4.67

LogS: -4.88

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(2,6-dichlorophenyl)-7-(dimethylamino)-4H-chromene-3-carbonitrile

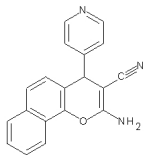
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(C(C(=C(O1)N)C#N)c1c(cccc1Cl)Cl)ccc(c2)N(C)C



ID: ST098243

Formula: C19H13N3O

MW: 299.33

LogP: 2.9

LogS: -4.24

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(4-pyridyl)-4H-benzo[h]chromene-3-carbonitrile

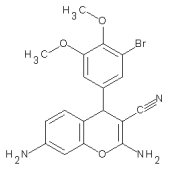
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(ccc3c2cccc3)C(C(=C(O1)N)C#N)c1ccncc1



ID: ST098244

Formula: C18H16BrN3O3

MW: 402.25

LogP: 2.94

LogS: -4.26

Acceptors: 3

Donors: 4

Oil: SOLID

IUPACNAME: 2,7-diamino-4-(3-bromo-4,5-dimethoxyphenyl)-4H-chromene-3-carbonitrile

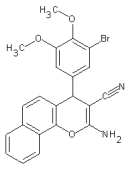
Rotation Bonds: 3

Lipinski: 4

N+O: 6

Chiral Centers: 1

Smiles: COc1c(c(cc(c1)C1c2c(OC(=C1C#N)N)cc(cc2)N)Br)OC



ID: ST098245

Formula: C22H17BrN2O3

MW: 437.29

LogP: 5.1

LogS: -5.24

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(3-bromo-4,5-dimethoxyphenyl)-4H-benzo[h]chromene-3-carbonitrile

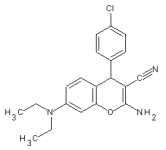
Rotation Bonds: 3

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: c12c(ccc3c2cccc3)C(C(=C(O1)N)C#N)c1cc(c(c(c1)Br)OC)OC



ID: ST098246

Formula: C20H20ClN3O

MW: 353.85

LogP: 5.08

LogS: -5.08

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(diethylamino)-4-(4-chlorophenyl)-4H-chromene-3-carbonitrile

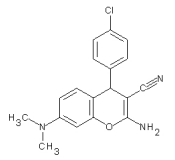
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c1(ccc(cc1)C1c2c(OC(=C1C#N)N)cc(cc2)N(CC)CC)Cl



ID: ST098247

Formula: C18H16ClN3O

MW: 325.8

LogP: 4.17

LogS: -4.65

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(dimethylamino)-4-(4-chlorophenyl)-4H-chromene-3-carbonitrile

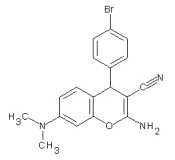
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(C)C)C(C(=C(O1)N)C#N)c1ccc(cc1)Cl



ID: ST098248

Formula: C18H16BrN3O

MW: 370.25

LogP: 4.35

LogS: -4.73

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(dimethylamino)-4-(4-bromophenyl)-4H-chromene-3-carbonitrile

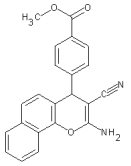
Rotation Bonds: 0

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(C)C)C(C(=C(O1)N)C#N)c1ccc(cc1)Br



ID: ST098249

Formula: C22H16N2O3

MW: 356.38

LogP: 4.72

LogS: -5.01

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: methyl 4-(2-amino-3-cyano-4H-benzo[h]chromen-4-yl)benzoate

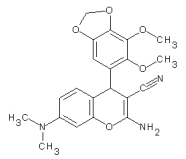
Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: c12c(ccc3c2cccc3)C(C(=C(O1)N)C#N)c1ccc(cc1)C(OC)=O



ID: ST098250

Formula: C21H21N3O5

MW: 395.41

LogP: 2.52

LogS: -4.39

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(6,7-dimethoxy(2H-benzo[d]1,3-dioxolan-5-yl))-7-(dimethylamino)-4H-c hromen

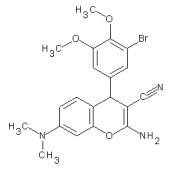
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(C)C)C(C(=C(O1)N)C#N)c1cc2c(c(c1OC)OC)OCO2



ID: ST098251

Formula: C20H20BrN3O3

MW: 430.3

LogP: 4.03

LogS: -4.85

Acceptors: 3

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(dimethylamino)-4-(3-bromo-4,5-dimethoxyphenyl)-4H-chromene-3-carbon itril

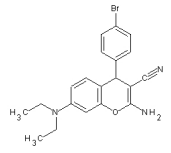
Rotation Bonds: 3

Lipinski: 4

N+O: 6

Chiral Centers: 1

Smiles: COc1c(c(cc(c1)C1c2c(OC(=C1C#N)N)cc(cc2)N(C)C)Br)OC



ID: ST098252

Formula: C20H20BrN3O

MW: 398.3

LogP: 5.26

LogS: -5.16

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(diethylamino)-4-(4-bromophenyl)-4H-chromene-3-carbonitrile

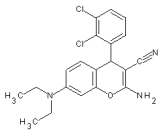
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c1(ccc(cc1)C1c2c(OC(=C1C#N)N)cc(cc2)N(CC)CC)Br



ID: ST098253

Formula: C20H19Cl2N3O

MW: 388.3

LogP: 5.64

LogS: -5.33

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(2,3-dichlorophenyl)-7-(diethylamino)-4H-chromene-3-carbonitrile

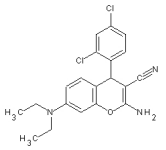
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c1ccc(c(c1Cl)Cl)C1c2c(OC(=C1C#N)N)cc(cc2)N(CC)CC



ID: ST098254

Formula: C20H19Cl2N3O

MW: 388.3

LogP: 5.57

LogS: -5.31

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(2,4-dichlorophenyl)-7-(diethylamino)-4H-chromene-3-carbonitrile

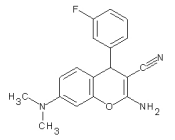
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c1(ccc(c(c1)Cl)C1c2c(OC(=C1C#N)N)cc(cc2)N(CC)CC)Cl



ID: ST098255

Formula: C18H16FN3O

MW: 309.34

LogP: 3.63

LogS: -4.41

Acceptors: 1

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(dimethylamino)-4-(3-fluorophenyl)-4H-chromene-3-carbonitrile

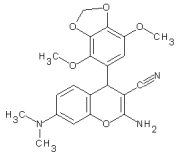
Rotation Bonds: 1

Lipinski: 4

N+O: 4

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(C)C)C(C(=C(O1)N)C#N)c1cc(ccc1)F



ID: ST098256

Formula: C21H21N3O5

MW: 395.41

LogP: 2.44

LogS: -4.36

Acceptors: 5

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-4-(4,7-dimethoxy(2H-benzo[d]1,3-dioxolan-5-yl))-7-(dimethylamino)-4H-c hromen

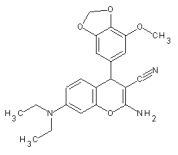
Rotation Bonds: 3

Lipinski: 4

N+O: 8

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(C)C)C(C(=C(O1)N)C#N)c1c(c2c(c(c1)OC)OCO2)OC



ID: ST098257

Formula: C22H23N3O4

MW: 393.44

LogP: 3.48

LogS: -4.73

Acceptors: 4

Donors: 2

Oil: SOLID

IUPACNAME: 2-amino-7-(diethylamino)-4-(7-methoxy(2H-benzo[d]1,3-dioxolan-5-yl))-4H-chrome ne-3-c

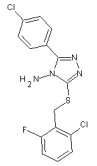
Rotation Bonds: 4

Lipinski: 4

N+O: 7

Chiral Centers: 1

Smiles: c12c(ccc(c2)N(CC)CC)C(C(=C(O1)N)C#N)c1cc2c(c(c1)OC)OCO2



ID: ST098258

Formula: C15H11Cl2FN4S

MW: 369.25

LogP: 5.65

LogS: -5.07

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: 3-[(6-chloro-2-fluorophenyl)methylthio]-5-(4-chlorophenyl)-1,2,4-triazole-4-yl amine

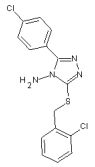
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1(c(nnc1SCc1c(F)cccc1Cl)c1ccc(cc1)Cl)N



ID: ST098259

Formula: C15H12Cl2N4S

MW: 351.26

LogP: 5.73

LogS: -5.08

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: 5-(4-chlorophenyl)-3-[(2-chlorophenyl)methylthio]-1,2,4-triazole-4-ylamine

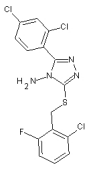
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: n1(c(nnc1SCc1c(Cl)cccc1)c1ccc(cc1)Cl)N



ID: ST098260

Formula: C15H10Cl3FN4S

MW: 403.69

LogP: 6.12

LogS: -5.29

Acceptors: 0

Donors: 2

Oil: SOLID

IUPACNAME: 3-(2,4-dichlorophenyl)-5-[(6-chloro-2-fluorophenyl)methylthio]-1,2,4-triazole- 4-ylamine

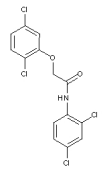
Rotation Bonds: 4

Lipinski: 3

N+O: 4

Chiral Centers: 0

Smiles: c1(n(c(SCc2c(F)cccc2Cl)nn1)N)c1c(cc(cc1)Cl)Cl



ID: ST098261

Formula: C14H9Cl4NO2

MW: 365.04

LogP: 4.79

LogS: -4.72

Acceptors: 2

Donors: 1

Oil: SOLID

IUPACNAME: N-(2,4-dichlorophenyl)-2-(2,5-dichlorophenoxy)acetamide

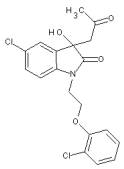
Rotation Bonds: 3

Lipinski: 4

N+O: 3

Chiral Centers: 0

Smiles: N(c1c(cc(cc1)Cl)Cl)C(=O)COc1cc(Cl)ccc1Cl



ID: ST098262

Formula: C19H17Cl2NO4

MW: 394.25

LogP: 3.23

LogS: -4.58

Acceptors: 4

Donors: 1

Oil: SOLID

IUPACNAME: 5-chloro-1-[2-(2-chlorophenoxy)ethyl]-3-hydroxy-3-(2-oxopropyl)indolin-2-one

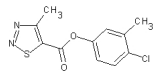
Rotation Bonds: 7

Lipinski: 4

N+O: 5

Chiral Centers: 1

Smiles: C1(C(c2c(ccc(c2)Cl)N1CCOc1c(Cl)cccc1)(CC(=O)C)O)=O



ID: ST098263

Formula: C11H9ClN2O2S

MW: 268.72

LogP: 4.24

LogS: -4.34

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 4-chloro-3-methylphenyl 4-methyl-1,2,3-thiadiazole-5-carboxylate

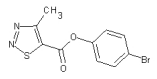
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(C(Oc2cc(C)c(cc2)Cl)=O)c(nns1)C



ID: ST098264

Formula: C10H7BrN2O2S

MW: 299.15

LogP: 3.75

LogS: -4.14

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 4-bromophenyl 4-methyl-1,2,3-thiadiazole-5-carboxylate

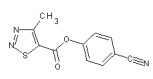
Rotation Bonds: 2

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(C(Oc2ccc(cc2)Br)=O)c(nns1)C



ID: ST098265

Formula: C11H7N3O2S

MW: 245.26

LogP: 2.51

LogS: -3.75

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 4-cyanophenyl 4-methyl-1,2,3-thiadiazole-5-carboxylate

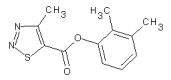
Rotation Bonds: 2

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: c1(C(Oc2ccc(C#N)cc2)=O)c(nns1)C



ID: ST098266

Formula: C12H12N2O2S

MW: 248.31

LogP: 4.25

LogS: -4.35

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 2,3-dimethylphenyl 4-methyl-1,2,3-thiadiazole-5-carboxylate

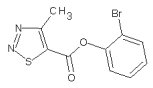
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(C(Oc2c(c(C)ccc2)C)=O)c(nns1)C



ID: ST098267

Formula: C10H7BrN2O2S

MW: 299.15

LogP: 3.73

LogS: -4.14

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 2-bromophenyl 4-methyl-1,2,3-thiadiazole-5-carboxylate

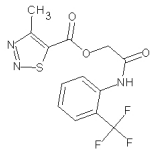
Rotation Bonds: 3

Lipinski: 4

N+O: 4

Chiral Centers: 0

Smiles: c1(C(Oc2c(Br)cccc2)=O)c(nns1)C



ID: ST098268

Formula: C13H10F3N3O3S

MW: 345.3

LogP: 2.65

LogS: -3.95

Acceptors: 3

Donors: 1

Oil: SOLID

IUPACNAME: {N-[2-(trifluoromethyl)phenyl]carbamoyl}methyl 4-methyl-1,2,3-thiadiazole-5-ca rboxylate

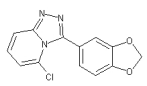
Rotation Bonds: 4

Lipinski: 4

N+O: 6

Chiral Centers: 0

Smiles: c1(c(nns1)C)C(OCC(Nc1c(C(F)(F)F)cccc1)=O)=O



ID: ST098269

Formula: C13H8ClN3O2

MW: 273.68

LogP: 2.72

LogS: -3.95

Acceptors: 2

Donors: 0

Oil: SOLID

IUPACNAME: 5-(5-chloro-4-hydro-1,2,4-triazolo[4,5-a]pyridin-3-yl)-2H-benzo[d]1,3-dioxolan e

Rotation Bonds: 1

Lipinski: 4

N+O: 5

Chiral Centers: 0

Smiles: n12c(nnc1cccc2Cl)c1cc2OCOc2cc1