



Formula: C₄H₄N₂OS

MW: 128.15

CAS: 141-90-2

TNP NUMBER: TNP00590

MDL NUMBER: MFCD00044203

IUPAC: 2-sulfanylpyrimidin-4-ol

Smiles: n1c(nccc1O)S

Occurs in seeds of Brassica, Cruciferae

THERAPEUTIC CATEGORY: Treatment of hyperthyroidism; angina pectoris; congestive heart failure

ACCEPTORS: 1

DONORS: 1

ROTATION BONDS: 2

N+O: 3

Chiral Centers: 0

LogP: -0.85

LogS: -2.09

LIPINSKI: 4

Synonyms:

4-HYDROXY-2-MERCAPTOPYRIMIDINE;4-HYDROXY-2-THIOPYRIMIDINE;2-MERCAPTO-4-PYRIMIDONE;2-MERCAPTO-4-HYDROXYPYRIMIDINE;2-THIOURACIL;2,3-dihydro-2-thioxo-4(1h)-pyrimidinone;DERACIL;2,3-dihydro-2-thioxo-4(1h)-pyrimidinon

CAS:141-90-2

MF:C4H4N2OS

MW:128.15

EINECS:205-508-8

Product Categories:PYRIMIDINE;FINE Chemical & INTERMEDIATES;Pyridines, Pyrimidines, Purines and Pteredines;Heterocyclic Compounds;Nucleic acids 2-Thiouracil

Chemical Properties: mp >300 C(lit.) storage temp. 2-8C Water Solubility 0.5 g/L Merck 14,9366 BRN 112227

CAS DataBase Reference: 141-90-2(

CAS DataBase Reference:) NIST Chemistry Reference2-Thiouracil(141-90-2) EPA Substance Registry System4(1H)-Pyrimidinone, 2,3-dihydro-2-thioxo-(141-90-2) Xn,T Risk Statements 40-45-20/21/22 Safety Statements 36/37-53-45 WGK Germany 3 RTECS YR1575000 HS Code 29335995 Hazardous Substances Data141-90-2(Hazardous Substances Data) 4-Hydroxy-2-mercaptopyrimidine 2-Thiouracil

Usage And Synthesis:

Chemical Properties: white to cream fine crystalline powder 2-Thiouracil

