



Formula: C₂₀H₂₄N₈O₆

MW: 472.46

Salt: H₂O

CAS: 133073-73-1

MDL NUMBER: MFCD00150845

IUPAC: 2-[(4-[(2,4-diaminopteridin-6-yl)methyl]methylamino)phenyl]carbonylamino]pentanedioic acid, hydrate

Smiles: Nc1c2c(ncc(n2)CN(C)c2ccc(cc2)C(NC(CCC(=O)O)C(=O)O)=O)nc(n1)N.O

Anticancer Drug

THERAPEUTIC CATEGORY: Antineoplastic

ACCEPTORS: 6

DONORS: 9

ROTATION BONDS: 9

N+O: 14

Chiral Centers: 1

LogP: -2.63

LogS: -2.68

LIPINSKI: 3

Synonyms:

METHOTREXATE; METHYLAMINOPTERIN; METHYLAMINOPTERINE; ANTIFOLAN; L-(+)-AMETHOPTERIN; 4-AMINO-N 10-METHYLPTEROYL-L-GLUTAMIC ACID; 4-AMINO-10-METHYLPTEROYLGLUTAMIC ACID; (+)-4-AMINO-10-METHYLFOLIC ACID

CAS:59-05-2

MF:C20H22N8O5

MW:454.44

EINECS:200-413-8

Product Categories: Aromatic Esters; Antibiotics for Research and Experimental Use; Antitumors for Research and Experimental Use; Biochemistry; Others (Antibiotics for Research and Experimental Use); Intermediates & Fine Chemicals; Pharmaceuticals; API's; Antitumour Methotrexate

Chemical Properties: mp 195C storage temp. -20C solubility H2O: insoluble form powder
Water Solubility Insoluble.