



Formula: C<sub>20</sub>H<sub>22</sub>N<sub>8</sub>O<sub>5</sub>

MW: 454.45

CAS: 51865-79-3

MDL NUMBER: MFCD00599529

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

Smiles: c1(nc(c2nc(CN(c3ccc(C(N[C@@H](CCC(=O)O)C(=O)O)=O)cc3)C)cnc2n1)N)N

Anticancer Drug. toxic antimetabolite that limits cellular reproduction by acting as an antagonist to folic acid; used to treat certain cancers and psoriasis and rheumatoid arthritis

THERAPEUTIC CATEGORY: Antineoplastic

ACCEPTORS: 5

DONORS: 7

ROTATION BONDS: 7

N+O: 13

Chiral Centers: 1

LogP: -1.26

LogS: -3.15

LIPINSKI: 3

Synonyms: D-AMETHOPTERIN HYDRATE, 95;L-Glutamic acid,  
N-4-(2,4-diamino-6-pteridiny)methylmethylaminobenzoyl-, monohydrate

CAS:6745-93-3

MF:C20H22N8O5

MW:0

EINECS:257-482-2

Product Categories: D-AMETHOPTERIN HYDRATE, 95

Chemical Properties: mp 195 C (dec.)(lit.) T Risk Statements 46-60-61-25-36/37/38 Safety  
Statements 53-22-26-36/37/39-45 RIDADR UN 1544 6.1/PG 3 RTECS MA1224000  
D-AMETHOPTERIN HYDRATE, 95

Usage And Synthesis: D-AMETHOPTERIN HYDRATE, 95

