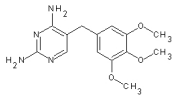

Formula: C14H18N4O3

MW: 290.32

CAS: 738-70-5

MDL NUMBER: MFCD00036761

IUPAC: 5-[(3,4,5-trimethoxyphenyl)methyl]pyrimidine-2,4-diamine

Smiles: c1(ncc(c(n1)N)Cc1cc(c(c(c1)OC)OC)OC)N

THERAPEUTIC CATEGORY: Antibacterial

REFERENCE: Cited Reference 1. D.P. Baccanari, et al. J. Biol. Chem. 264, 1100, (1989) 2. N.J. Prendergast, et al. Biochemistry 28, 4645, (1989) Reference Schweitzer, B.I., Dihydrofolate reductase as a therapeutic target. FASEB J. 4, 2441, (1990) abstract Periti, P., Evolution of the bacterial dihydrofolate reductase inhibitors. J. Antimicrob. Chemother. 36, 887, (1995) abstract Merck Merck 13,9782

ACCEPTORS: 3

DONORS: 4

ROTATION BONDS: 3

N+O: 7

Chiral Centers: 0

LogP: 1.65

LogS: -3.59

LIPINSKI: 4

Monograph Number: 0009782

Title: Trimethoprim

CAS Registry Number: 738-70-5

CAS Name: 5-[(3,4,5-Trimethoxyphenyl)methyl]-2,4-pyrimidinediamine

Additional Names: 2,4-diamino-5-(3,4,5-trimethoxybenzyl)pyrimidine

Trademarks: Instalac (Virbac); Monotrim (Duphar); Proloprim (Wellcome); Syraprim (Wellcome); Tiempe (DDSA); Trimanyl (Tosse); Trimogal (Lagap); Trimopan (Berk); Trimpex (Roche); Uretrim (Bastian); Wellcoprim (Wellcome)

Molecular Formula: C14H18N4O3

Molecular Weight: 290.32.

Percent Composition: C 57.92%, H 6.25%, N 19.30%, O 16.53%

Literature References: Prepn from guanidine and b-ethoxy-3,4,5-trimethoxybenzylbenzalnitrile: Stenbuck, Hood, US 3049544 (1962 to Burroughs Wellcome); Hoffer, US 3341541 (1967 to Hoffmann-La Roche). Improved synthesis: B. Roth et al., J. Med. Chem. 23, 379, 535 (1980). Toxicity data: Yamamoto et al., Chemotherapy (Tokyo) 21, 187 (1973). Review: Burchall in Antibiotics vol. 3, J. W. Corcoran, F. E. Hahn, Eds. (Springer-Verlag, New York, 1975) pp 304-320. Comprehensive description: G. J. Manius, Anal. Profiles Drug Subs. 7, 445-475 (1978). Review of antibacterial activity, pharmacokinetics and therapeutic use: R. N. Brogden et al., Drugs 23, 405-430 (1982).

Properties: White to cream, bitter crystalline powder, mp 199-203. Soly in g/100 ml at 25: DMAC 13.86; benzyl alcohol 7.29; propylene glycol 2.57; chloroform 1.82; methanol 1.21; water 0.04; ether 0.003; benzene 0.002. pKa 6.6. LD50 orally in mice: 7000 mg/kg (Yamamoto).

Melting point: mp 199-203

pKa: pKa 6.6

Toxicity data: LD50 orally in mice: 7000 mg/kg (Yamamoto)

NOTE: See Sulfamethoxazole, Sulfadiazine, Sulfametrole, Sulfamoxole, and Sulfalene for lists of trade names of mixtures with Trimethoprim.

Therap-Cat: Antibacterial.

Therap-Cat-Vet: Antibacterial.

Synonyms:
abaprim;5-((3,4,5-trimethoxyphenyl)methyl)-2,4-pyrimidinediamine;5-(3,4,5-trimethoxybenzyl)-2,4-diaminopyrimidine;5-(3,4,5-TRIMETHOXYBENZYL)PYRIMIDINE-2,4-DIYLAMINE;2,4-DIAMINO-5-(3,4,5-TRIMETHOXYBENZYL)PYRIMIDE;2,4-DIAMINO-5-(3',4',5'-TRIMETHOXYBENZYL)PYRIMIDINE;2,4-DIAMINO-5-(3,4,5-TRIMETHOXYBENZYL)PYRIMIDINE;TRIMETOPRIM

CAS:738-70-5

MF:C14H18N4O3

MW:290.32

EINECS:212-006-2

Product Categories:Pharmaceutical;Inhibitors;Intermediates & Fine Chemicals;Pharmaceuticals;Peptide Synthesis/Antibiotics Trimethoprim

Chemical Properties: mp 199-203 C storage temp. 2-8C solubility DMSO: soluble form white powder Water Solubility