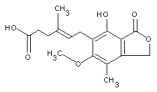

Formula: C17H20O6

MW: 320.34

CAS: 24280-93-1

TNP NUMBER: TNP00198

MDL NUMBER: MFCD00036814

IUPAC: (4E)-6-(4-hydroxy-6-methoxy-7-methyl-3-oxohydroisobenzofuran-5-yl)-4-methylhex-4-enoic acid

Smiles: c12c(c(C)c(c(c1O)CC=C(CCC(=O)O)C)OC)COC2=O

ACCEPTORS: 6

DONORS: 2

ROTATION BONDS: 8

N+O: 6

Chiral Centers: 0

LogP: 3.8

LogS: -4.34

LIPINSKI: 4

Monograph Number: 0006352

Title: Mycophenolic Acid

CAS Registry Number: 24280-93-1

CAS Name:
(4E)-6-(1,3-Dihydro-4-hydroxy-6-methoxy-7-methyl-3-oxo-5-isobenzofuranyl)-4-methyl-4-hexen oic acid

Additional Names: 6-(4-hydroxy-6-methoxy-7-methyl-3-oxo-5-phthalanyl)-4-methyl-4-hexenoic acid

Trademarks: Melbex (Lilly)

Molecular Formula: C17H20O6

Molecular Weight: 320.34.

Percent Composition: C 63.74%, H 6.29%, O 29.97%

Literature References: Antibiotic produced by Penicillium brevi-compactum, P. stoloniferum and related spp. Selectively inhibits lymphocyte proliferation by blocking inosine monophosphate dehydrogenase (IMPDH), an enzyme involved in the de novo synthesis of purine nucleotides. Isoln: C. L. Alsberg, O. F. Black, USDA Bur. Plant Ind. Bull. 270, 7 (1912), C.A. 7, 3992 (1913); P. W. Clutterbuck et al., Biochem. J. 26, 1441 (1932); and antimicrobial activity: H. W. Florey et al., Lancet 1, 46 (1946). Structure: J. H. Birkinshaw et al., Biochem. J. 50, 630 (1952); W. R. Logan, G. T. Newbold, J. Chem. Soc. 1957, 1946. Total synthesis: A. J. Birch, J. J. Wright, Aust. J. Chem. 22, 2635 (1969). Biosynthesis: L. Canonica et al., J. Chem. Soc. Perkin Trans. 1 1972, 2639. Antitumor activity: R. H. Williams et al., Antimicrob. Agents Chemother. 1968, 229; S. B. Carter et al., Nature 223, 848 (1969). Immunosuppressive effect: A. Mitsui, S. Suzuki, J. Antibiot. 22, 358 (1969). Prepn of mofetil ester prodrug: P. H. Nelson et al., US 4753935 (1988 to Syntex); and bioavailability: W. A. Lee et al., Pharm. Res. 7, 161 (1990). Mechanism of action: A. C. Allison, E. M. Eugui, Transplant. Proc. 26, 3205 (1994); J. T. Ransom, Ther. Drug Monit. 17, 681 (1995). HPLC determn in plasma: S. Li, R. W. Yatscoff, Transplant. Proc. 28, 938 (1996). Pharmacokinetics: R. E. S. Bullingham et al., ibid. 925. Clinical trial in renal transplantation: P. A. Keown et al., Transplantation 61, 1029 (1996). Reviews: D. O. Taylor et al., J. Heart Lung Transplant. 13, 571-582 (1994); J. J. Lipsky, Lancet 348, 1357-1359 (1996).

Properties: Needles from hot water, mp 141. pKa 4.5. Partition coefficient (n-octanol/water): 570 (pH 2); 1.6 (pH 7.4). Almost insol in cold water. Sol in alcohol. LD50 in mice, rats (mg/kg): 2500, 700 orally; 550, 450 i.v. (Carter).

Melting point: mp 141

pKa: pKa 4.5

Log P: Partition coefficient (n-octanol/water): 570 (pH 2); 1.6 (pH 7.4)

Toxicity data: LD50 in mice, rats (mg/kg): 2500, 700 orally; 550, 450 i.v. (Carter)

Derivative Type: 2-(4-Morpholinyl)ethyl ester

CAS Registry Number: 128794-94-5

Additional Names: Mycophenolate mofetil

Manufacturers' Codes: RS-61443

Trademarks: Cellcept (Roche)

Molecular Formula: C23H31NO7

Molecular Weight: 433.49.

Percent Composition: C 63.73%, H 7.21%, N 3.23%, O 25.84%

Properties: White to off-white crystalline powder, mp 93-94. pKa 5.6. Partition coefficient (n-octanol/water): 0.0085 (pH 2); 238 (pH 7.4). Sol in acetone, methanol. Slightly sol in water; sparingly sol in ethanol.

Melting point: mp 93-94

pKa: pKa 5.6

Log P: Partition coefficient (n-octanol/water): 0.0085 (pH 2); 238 (pH 7.4)

Therap-Cat: Immunosuppressant.

Synonyms:
4-methyl-5-methoxy-7-hydroxy-6-(5-carboxy-3-methylpent-2-en-1-yl)-phthalide;6-(5-carboxy-3-

methyl-2-pentenyl)-7-hydroxy-5-methoxy-4-methyl-phthalid;lilly-68618;melbex;micofenolicoacid o;nsc-129185;(4E)-6-(1,3-DIHYDRO-4-HYDROXY-6-METHOXY-7-METHYL-3-OXO-5-ISOBEN ZOFURANYL)-4-METHYL-4-HEXENOIC ACID;6-(4-HYDROXY-6-METHOXY-7-METHYL-3-OXO-5-PHTHALANYL)-4-METHYL-4-HEXA NOIC ACID

CAS:24280-93-1

MF:C17H20O6

MW:320.34

EINECS:246-119-3

Product Categories:Active Pharmaceutical Ingredients;Aromatics Compounds;Aromatics;Inhibitors;Intermediates & Fine Chemicals;Pharmaceuticals Mycophenolic acid

Chemical Properties: mp 141C storage temp. 2-8C solubility methanol: 50 mg/mL, clear, colorless to faintly yellow form powder Merck 13,6352

CAS DataBase Reference: 24280-93-1(

CAS DataBase Reference: ) Xn Risk Statements 22-61-40 Safety Statements 53-45-36/37 RIDADR 2811 WGK Germany 3 RTECS MP8050000 F 10 HazardClass 6.1(b) PackingGroup III Mycophenolic acid Mycophenolic acid

Usage And Synthesis:

Chemical Properties: White to Off-White Powder UsageAn antibiotic produced by Penicillium brevi-compactum, P. Stoloniferum and related spp. A selective inhibitor of lymphocyte proliferation by blocking inosine monophosphate dehydrogenase, an enzyme involved in the de novo synthesis of purine nucleot Biological ActivityImmunosuppressive agent with antiviral and antitumor effects in vitro and in vivo . Potently inhibits inosine monophosphate dehydrogenase, thus inhibiting de novo GTP synthesis leading to decreased RNA and DNA synthesis. Reversibly inhibits proliferation of T and B lymphocytes and antibody formation. Mycophenolic acid