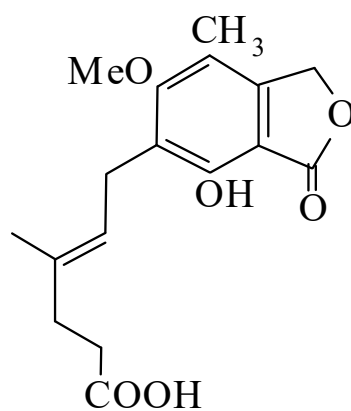




>>Entry Name: Mycophenolic acid, BAN, INN, USAN

Synonym(s): 6-(1,3-Dihydro-4-hydroxy-6-methoxy-7-methyl-3-oxo-5-isobenzofuranyl)-4-methyl-4-hexenoic acid, 9CI. Melbex. Lilly 68618. NSC 129185



CAS Registry Number: 24280-93-1

Related CAS Registry Numbers(s): 115007-34-6

Molecular Formula: C₁₇H₂₀O₆

Molecular Weight: 320.341

Accurate Mass: 320.12599

Percentage Composition: C 63.74%; H 6.29%; O 29.97%

Biological Source: Metab. of *Penicillium brevi-compactum*, *Penicillium stoloniferum* and other *Penicillium* spp.

Use/Importance: Shows exp. antineoplastic and antiviral props. Useful in treating psoriasis and leishmaniasis. Shows immunosuppressant props., used in the prophylaxis of acute kidney rejection

Physical Description: Needles (H₂O)

Melting Point: Mp 141°

Solubility: BERDY SOL: Sol. MeOH, Et₂O, CHCl₃; fairly sol. C₆H₆, toluene; poorly sol. H₂O

Calculated Log P Data: Log P 3.38 (uncertain value) (calc)

UV: [base] λ_{max} (solvent not reported) (Derep) [neutral] λ_{max} 249 (ε 10300); 305 (ε 5300) (EtOH) (Derep) [neutral] λ_{max} 250 (ε 8080); 305 (ε 4300) (EtOH) (Berdy)

Hazard & Toxicity: LD₅₀ (rat, orl) 352 mg/kg. Exp. reprod. effects ; BERDY HAZD : LD₅₀ (mus, ipr) 973 mg/kg , LD₅₀ (mus, orl) 2000 - 4000 mg/kg

Fluka: 70018

Sigma: M3536

>>Derivative: Et ester

CAS Registry Number: 32483-51-5

Molecular Formula: C₁₉H₂₄O₆

Molecular Weight: 348.395

Accurate Mass: 348.15729

Percentage Composition: C 65.50%; H 6.94%; O 27.55%

Biological Source: Prod. by *Penicillium brevi-compactum*

Physical Description: Cryst.

Melting Point: Mp 88-90°

UV: [neutral] λ_{max} 303 (ε 4700) (MeOH) [neutral] λ_{max} 303 (ε 4700) (MeOH) (Berdy) [base] λ_{max} 341 (ε 7900) (NAOH) (Berdy)

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

Synonym(s): Mycophenolate mofetil, USAN. CellCept. RS 61443

CAS Registry Number: 128794-94-5

Extra CAS Registry Numbers(s): 116680-01-4

Molecular Formula: C₂₃H₃₁NO₇

Molecular Weight: 433.5

Accurate Mass: 433.210054

Percentage Composition: C 63.73%; H 7.21%; N 3.23%; O 25.84%

Use/Importance: Antiarthritic, immunosuppressant used in kidney transplant rejection

Development Status: Launched in 1995 (US)

Melting Point: Mp 93-94°

References: