Leflunomide c12h9f3n2o2 structure

Contents

Molecular Formula	$C_{12}H_9F_3N_2O_2$
Average mass	270. 207 Da
Density	1. 4±0. 1 g/cm ^{3}
Boiling Point	289. 3±40. 0 °C at 760 mmHg
Flash Point	128. 8±27. 3 °C
Molar Refractivity	61. 0±0. 3 cm ^{3}
Polarizability	24. 2±0. 5 10^{-24} cm ^{3}
Surface Tension	40. 6±3. 0 dyne/cm
Molar Volume	194. 1±3. 0 cm ^{3}

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

166. 5 °CLKT

Labs[L1817]

165. 5 °CJean-Claude

Bradley Open Melting

Point Dataset16294

166. 5 °CJean-Claude

Bradley Open Melting

Point Dataset21795

166 °CBiosynthQ-

201289

153-156

°CLabNetworkLN00176

083

Experimental Flash Point:

129 °CBiosynthQ-

201289

- **Experimental Gravity:**

  129 g/mLBiosynthQ-

  201289

- **Experimental Solubility:**

  10 mM in

  H2OMedChem

  ExpressHY-B0083

  DMSO 54 mg/mL;

  MedChem ExpressHY-

  B0083

  Soluble in DMSO or

  methanol. LKT

  Labs[L1817]

  Soluble to 100 mM in

  ethanol and to 100 mM

  in DMSOTocris

  Bioscience2228

- Miscellaneous

  - **Safety:**

    22-36/37/38LKT

    Labs[L1817]

DangerBiosynthQ-

201289

GHS06BiosynthQ-

201289

H301; H315; H319;

H335BiosynthQ-

201289

H302 H315 H335

H319LKT Labs[L1817]

IRRITANTMatrix

Scientific078298

P261; P301+P310;

P305+P351+P338Biosy

nthQ-201289

Xn, XiLKT Labs[L1817]

- **Target Organs:**

Protein-tyrosine kinase

2 antagonist; AhR

agonist;

Dehydrogenase

inhibitorTargetMolT115

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- **Drug Status:**

approvedBIONET-Key OrganicsKS-1076

- **Compound Source:**

syntheticMicrosource[01503927]

synthetic; SU-101; HWA-486Microsource[01503927]

- **Bio Activity:**

DehydrogenasesTocris Bioscience2228

Dihydroorotate dehydrogenase inhibitorTocris Bioscience2228

EnzymeTargetMolT1159

EnzymesTocris Bioscience2228

Inhibitor of dihydroorotate dehydrogenase (IC50 = 2. 5 ? M). Inhibits de novo pyrimidine synthesis in human T cells in vitro; also inhibits lymphocyte proliferation. Exhibits efficacy in several animalmodels of autoimmune disease, arthritis and graft rejection. Active metabolite, teriflunomide (A77 1726, Cat. No. 5069), also available. Tocris Bioscience2228

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Leflunomide(SU101; HWA486; RS-34821) is a disease-modifying antirheumatic drug, which is a pyrimidine synthesis inhibitor. MedChem Express

Leflunomide(SU101;

HWA486; RS-34821) is a disease-modifying antirheumatic drug, which is a pyrimidine synthesis inhibitor.; IC50 Value: ; Target: pyrimidine synthesis; Leflunomide is a pyrimidine synthesis inhibitor belonging to the DMARD (disease-modifying antirheumatic drug) class of drugs.

MedChem ExpressHY-B0083

Other DehydrogenasesTocris Bioscience2228

OthersMedChem ExpressHY-B0083

Protein-tyrosine kinase 2; AhR; DHODHTargetMolT115

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Predicted data is generated using the ACD/Labs Percepta Platform – PhysChem Module

Density:	1. 4±0. 1 g/cm ^{3}
Boiling Point:	289. 3±40. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 6 mmHg at 25°C
Enthalpy of Vaporization:	52. 9±3. 0 kJ/mol
Flash Point:	128. 8±27. 3 °C
Index of Refraction:	1. 541
Molar Refractivity:	61. 0±0. 3 cm ^{3}
#H bond acceptors:	4
#H bond donors:	1
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	0
ACD/LogP:	1. 95
ACD/LogD (pH 5. 5):	2. 20
ACD/BCF (pH 5. 5):	27. 82

ACD/KOC (pH 5. 5):	376. 21
ACD/LogD (pH 7. 4):	2. 20
ACD/BCF (pH 7. 4):	27. 81
ACD/KOC (pH 7. 4):	376. 18
Polar Surface Area:	55 Å ^{2}
Polarizability:	24. 2±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	40. 6±3. 0 dyne/cm
Molar Volume:	194. 1±3. 0 cm ^{3}

Predicted data is generated using the US Environmental Protection Agency's EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 2. 43Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 378. 79 (Adapted Stein & Brown method)Melting Pt (deg C): 155. 71 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 1. 25E-006 (Modified Grain method)Subcooled liquid VP: 2. 71E-005 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 152. 7log Kow used: 2. 43 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 23. 356 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 23E-010 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 910E-009 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 43 (KowWin est)Log Kaw used: -8. 299 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 10. 729Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 3633Biowin2 (Non-Linear Model) : 0. 0381Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 1. 9600 (months)Biowin4 (Primary Survey Model) : 3. 3204 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1696Biowin6

(MITI Non-Linear Model): 0. 0000Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 5807Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 00361 Pa (2. 71E-005 mm Hg)Log Koa (Koawin est): 10. 729Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00083 Octanol/air (Koa) model: 0. 0132 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0291 Mackay model : 0. 0623 Octanol/air (Koa) model: 0. 513 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 7. 3337 E-12 cm3/molecule-secHalf-Life = 1. 458 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 17. 502 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 0457 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2323Log Koc: 3. 366 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Rate constants can NOT be estimated for this structure! Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 1. 172 (BCF = 14. 88)log Kow used: 2. 43 (estimated)Volatilization from Water: Henry LC: 1. 23E-010 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 7. 825E+006 hours (3. 26E+005 days)Half-Life from Model Lake : 8. 536E+007 hours (3. 557E+006 days)Removal In Wastewater Treatment: Total removal: 2. 91 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 81 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 000753 35 1000 Water 15. 6 1. 44e+003 1000 Soil 84. 3 2. 88e+003 1000 Sediment 0. 117 1. 3e+004 0 Persistence Time: 2. 31e+003 hr

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- 1-Click Scaffold Hop