

# [Leflunomide c12h9f3n2o2 structure](https://assignbuster.com/leflunomide-c12h9f3n2o2-structure/)

Contents

* Bio Activity:

|  |  |
| --- | --- |
| Molecular Formula  | C 12 H 9 F 3 N 2 O 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  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* 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 °CLabNetworkLN00176083  |

## Experimental Flash Point:

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| --- |
| 129 °CBiosynthQ-201289  |

## Experimental Gravity:

|  |
| --- |
| 129 g/mLBiosynthQ-201289  |

## Experimental Solubility:

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| --- |
| 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+P338BiosynthQ-201289  |
| Xn, XiLKT Labs[L1817]  |

## Target Organs:

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| Protein-tyrosine kinase 2 antagonist; AhR agonist; Dehydrogenase inhibitorTargetMolT1159  |

## Drug Status:

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| --- |
| 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  |
| 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 animal models of autoimmune disease, arthritis and graft rejection. Active metabolite, teriflunomide (A77 1726, Cat. No. 5069), also available. Tocris Bioscience2228  |
| 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; DHODHTargetMolT1159  |

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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