

# [Labetalol c19h24n2o3 structure](https://assignbuster.com/labetalol-c19h24n2o3-structure/)

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* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 19 H 24 N 2 O 3  |
| Average mass  | 328. 405 Da  |
| Density  | 1. 2±0. 1 g/cm 3  |
| Boiling Point  | 552. 7±50. 0 °C at 760 mmHg  |
| Flash Point  | 288. 1±30. 1 °C  |
| Molar Refractivity  | 94. 7±0. 3 cm 3  |
| Polarizability  | 37. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 55. 1±3. 0 dyne/cm  |
| Molar Volume  | 273. 6±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 195. 5 °CJean-Claude Bradley Open Melting Point Dataset16533, 17160  |
| 188 °CJean-Claude Bradley Open Melting Point Dataset16533, 17160, 21797  |

## Experimental Flash Point:

|  |
| --- |
| 288. 1 °CBiosynthQ-201273  |

## Experimental Gravity:

|  |
| --- |
| 288. 1 g/mLBiosynthQ-201273  |

* Miscellaneous

## Safety:

|  |
| --- |
| GHS07BiosynthQ-201273  |
| H302BiosynthQ-201273  |
| P261; P280; P302+P352; P304+P340; P305+P351+P338; P312BiosynthQ-201273  |
| WarningBiosynthQ-201273  |

## Therapeutical Effect:

|  |
| --- |
| Antihypertensive Agents, SympatholyticsSean Ekins  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 3004 (estimated with error: 89)NIST Spectramainlib\_248725, replib\_120430  |

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

|  |  |
| --- | --- |
| Density:  | 1. 2±0. 1 g/cm 3  |
| Boiling Point:  | 552. 7±50. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±1. 6 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 87. 7±3. 0 kJ/mol  |
| Flash Point:  | 288. 1±30. 1 °C  |
| Index of Refraction:  | 1. 609  |
| Molar Refractivity:  | 94. 7±0. 3 cm 3  |
| #H bond acceptors:  | 5  |
| #H bond donors:  | 5  |
| #Freely Rotating Bonds:  | 8  |
| #Rule of 5 Violations:  | 1  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 31  |
| ACD/LogD (pH 5. 5):  | -0. 27  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 00  |
| ACD/LogD (pH 7. 4):  | 0. 85  |
| ACD/BCF (pH 7. 4):  | 1. 00  |
| ACD/KOC (pH 7. 4):  | 9. 43  |
| Polar Surface Area:  | 96 Å 2  |
| Polarizability:  | 37. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 55. 1±3. 0 dyne/cm  |
| Molar Volume:  | 273. 6±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. 41Log Kow (Exper. database match) = 3. 09Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 533. 96 (Adapted Stein & Brown method)Melting Pt (deg C): 228. 46 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 3. 33E-013 (Modified Grain method)MP (exp database): 188 deg CSubcooled liquid VP: 1. 69E-011 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): 72. 9log Kow used: 3. 09 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 75267 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesPhenolsBenzyl AlcoholsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 63E-019 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 974E-015 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 3. 09 (exp database)Log Kaw used: -16. 567 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 19. 657Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 4125Biowin2 (Non-Linear Model) : 0. 9986Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6072 (weeks-months)Biowin4 (Primary Survey Model) : 3. 7281 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 1693Biowin6 (MITI Non-Linear Model): 0. 0482Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 1684Ready 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): 2. 25E-009 Pa (1. 69E-011 mm Hg)Log Koa (Koawin est ): 19. 657Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 33E+003 Octanol/air (Koa) model: 1. 11E+007 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1 Mackay model : 1 Octanol/air (Koa) model: 1 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 150. 6411 E-12 cm3/molecule-secHalf-Life = 0. 071 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 852 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 1 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5677Log Koc: 3. 754 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. 029 (BCF = 10. 7)log Kow used: 3. 09 (expkow database)Volatilization from Water: Henry LC: 6. 63E-019 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 6E+015 hours (6. 668E+013 days)Half-Life from Model Lake : 1. 746E+016 hours (7. 274E+014 days)Removal In Wastewater Treatment: Total removal: 6. 53 percentTotal biodegradation: 0. 13 percentTotal sludge adsorption: 6. 40 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 1. 33e-007 1. 7 1000 Water 12. 5 900 1000 Soil 87. 1 1. 8e+003 1000 Sediment 0. 349 8. 1e+003 0 Persistence Time: 1. 79e+003 hr

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