Labetalol c19h24n2o3 structure

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Molecular Formula	$C_{19}H_{24}N_2O_3$
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:**

    GHS07Biosynth

    Q-201273

    H302BiosynthQ-

    201273

    P261; P280;

    P302+P352;

P304+P340;

P305+P351+P3

38;

P312BiosynthQ-

201273

WarningBiosynt

hQ-201273

- **Therapeutical Effect:**

  Antihypertensiv

  e Agents,

  SympatholyticsS

  ean 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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