# Bemidone c15h21no3 structure

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\n[/toc]\n \n

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- Retention Index (Normal Alkane):

| | |
|---|---|
| Molecular Formula | $C_{15}H_{21}NO_3$ |
| Average mass | 263. 332 Da |
| Density | 1. 1±0. 1 g/cm $^3$ |
| Boiling Point | 384. 2±42. 0 °C at 760 mmHg |
| Flash Point | 186. 2±27. 9 °C |
| Molar Refractivity | 73. 1±0. 3 |

| | |
|---|---|
| | cm $^{3}$ |
| Polarizabilit y | 29. 0±0. 5 $10^{-24}$ cm $^{3}$ |
| Surface Tension | 43. 7±3. 0 dyne/cm |
| Molar Volume | 232. 7±3. 0 cm $^{3}$ |

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

      110 °CJean-

      Claude

      Bradley Open

      Melting Point

      Dataset2282

      3
- Gas Chromatography

- **Retention Index (Kovats):**

  2127

  (estimated

  with error:

  89)NIST

  Spectramainli

  b_58690

- **Retention Index (Normal Alkane):**

  2045

  (Program

  type: Ramp;

  Column cl...

  (show

  more)ass:

  Standard

  non-polar;

  Column type:

  Other; CAS

  no: 468564;

  Active phase:

  Methyl

  Silicone; Data

  type: Normal

  alkane RI;

  Authors:

Ardrey, R. E.; Moffat, A. C., Gas-liquid chromatographic retention indices of 1318 substances of toxicological interest on SE-30 or OV-1 stationary phase, J. Chromatogr., 220, 1981, 195-252.)NIST Spectranist ri

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

| | |
|---|---|
| Density: | 1. 1±0. 1 g/cm $^3$ |
| Boiling Point: | 384. 2±42. 0 °C at 760 mmHg |
| Vapour Pressure: | 0. 0±0. 9 mmHg at 25°C |

| | |
|---|---|
| Enthalpy of Vaporization: | 65. 8±3. 0 kJ/mol |
| Flash Point: | 186. 2±27. 9 °C |
| Index of Refraction: | 1. 541 |
| Molar Refractivity: | 73. 1±0. 3 $cm^3$ |
| #H bond acceptors: | 4 |
| #H bond donors: | 1 |
| #Freely Rotating Bonds: | 4 |
| #Rule of 5 Violations: | 0 |
| ACD/LogP: | 1. 61 |
| ACD/LogD (pH 5. 5): | -0. 31 |
| ACD/BCF (pH 5. 5): | 1. 00 |
| ACD/KOC (pH 5. 5): | 1. 72 |
| ACD/LogD (pH 7. 4): | 1. 37 |
| ACD/BCF (pH 7. 4): | 4. 96 |
| ACD/KOC (pH 7. 4): | 80. 61 |

| | |
|---|---|
| Polar Surface Area: | 50 Å $^{2}$ |
| Polarizability: | 29. 0±0. 5 10 $^{-24}$ cm $^{3}$ |
| Surface Tension: | 43. 7±3. 0 dyne/cm |
| Molar Volume: | 232. 7±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. 55Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 364. 54 (Adapted Stein & Brown method)Melting Pt (deg C): 133. 27 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 2. 17E-006 (Modified Grain method)MP (exp database): 110 deg CSubcooled liquid VP: 1. 48E-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): 5148log Kow used: 2. 55 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 23120 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesEstersPhenolsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 00E-012 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 461E-010 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 55 (KowWin est)Log Kaw used: -10. 388 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 12. 938Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5230Biowin2 (Non-Linear Model) : 0. 5772Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 3469 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2950 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4815Biowin6 (MITI Non-Linear Model): 0. 3345Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -1. 3154Ready 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. 00197 Pa (1. 48E-005 mm Hg)Log Koa (Koawin est ): 12. 938Kp (particle/gas partition coef. (m3/ug)): Mackay model : 0. 00152 Octanol/air (Koa) model: 2. 13 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 0521 Mackay model : 0. 108 Octanol/air (Koa) model: 0. 994 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 166. 6850 E-12 cm3/molecule-secHalf-Life = 0. 064 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 770 HrsOzone Reaction: No Ozone Reaction EstimationReaction With Nitrate Radicals May Be Important! Fraction sorbed to airborne particulates (phi): 0. 0802 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5897Log Koc: 3. 771 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 2. 680E-004 L/mol-secKb Half-Life at pH 8: 81. 939 years Kb Half-Life at pH 7: 819. 392 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log

BCF from regression-based method = 1. 262 (BCF = 18. 27)log Kow used: 2. 55 (estimated)Volatilization from Water: Henry LC: 1E-012 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 9. 501E+008 hours (3. 959E+007 days)Half-Life from Model Lake : 1. 036E+010 hours (4. 319E+008 days)Removal In Wastewater Treatment: Total removal: 3. 25 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 3. 14 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 8. 48e-006 1. 54 1000 Water 15. 6 900 1000 Soil 84. 3 1. 8e+003 1000 Sediment 0. 14 8. 1e+003 0 Persistence Time: 1. 67e+003 hr

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