

# [2-carbomethoxy-8-methyl-8-azabicyclo[3.2.1]oct-2-ene c10h15no2 structure](https://assignbuster.com/2-carbomethoxy-8-methyl-8-azabicyclo321oct-2-ene-c10h15no2-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 10 H 15 NO 2  |
| Average mass  | 181. 232 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 250. 2±20. 0 °C at 760 mmHg  |
| Flash Point  | 96. 9±12. 6 °C  |
| Molar Refractivity  | 49. 2±0. 3 cm 3  |
| Polarizability  | 19. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 37. 5±3. 0 dyne/cm  |
| Molar Volume  | 162. 9±3. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1313 (estimated with error: 89)NIST Spectramainlib\_367254, mainlib\_379439, replib\_124027, replib\_292774  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1337. 2 (Program type: Complex; Column… (show more)class: Standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: 5 min at 80 C; 80-160 C at 25 deg/min; hold at 160 C for 1 min; 160-275 C at 4 deg/min; hold at 275 C for 5 min; CAS no: 127379242; Active phase: DB-1; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Moore, J. M.; Casale, J. F., Lesser alkaloids of cocaine-bearing plants. Part 1: Nicotinoyl-, 2′-pyrroloyl and 2′- and 3′-furanoylecgonine methyl ester-isolation and mass spectral characterization of four new alkaloids of South American Erythroxylum coca Var. coca, J. Forensic Sci., 42(2), 1997, 246-255.)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:  | 250. 2±20. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 5 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 48. 8±3. 0 kJ/mol  |
| Flash Point:  | 96. 9±12. 6 °C  |
| Index of Refraction:  | 1. 515  |
| Molar Refractivity:  | 49. 2±0. 3 cm 3  |
| #H bond acceptors:  | 3  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 70  |
| ACD/LogD (pH 5. 5):  | -1. 14  |
| ACD/BCF (pH 5. 5):  | 1. 00  |
| ACD/KOC (pH 5. 5):  | 1. 00  |
| ACD/LogD (pH 7. 4):  | 0. 57  |
| ACD/BCF (pH 7. 4):  | 1. 10  |
| ACD/KOC (pH 7. 4):  | 24. 03  |
| Polar Surface Area:  | 30 Å 2  |
| Polarizability:  | 19. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 37. 5±3. 0 dyne/cm  |
| Molar Volume:  | 162. 9±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) = 1. 16Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 243. 08 (Adapted Stein & Brown method)Melting Pt (deg C): 47. 48 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0236 (Modified Grain method)Subcooled liquid VP: 0. 0379 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): 5. 63e+004log Kow used: 1. 16 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 42290 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: AcrylatesAliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 86E-008 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 9. 996E-008 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 16 (KowWin est)Log Kaw used: -5. 802 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 962Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6302Biowin2 (Non-Linear Model) : 0. 9082Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6841 (weeks-months)Biowin4 (Primary Survey Model) : 3. 5272 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 5229Biowin6 (MITI Non-Linear Model): 0. 3585Anaerobic 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): 5. 05 Pa (0. 0379 mm Hg)Log Koa (Koawin est ): 6. 962Kp (particle/gas partition coef. (m3/ug)): Mackay model : 5. 94E-007 Octanol/air (Koa) model: 2. 25E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 14E-005 Mackay model : 4. 75E-005 Octanol/air (Koa) model: 0. 00018 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 72. 5269 E-12 cm3/molecule-secHalf-Life = 0. 147 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 1. 770 HrsOzone Reaction: OVERALL Ozone Rate Constant = 7. 393750 E-17 cm3/molecule-secHalf-Life = 0. 155 Days (at 7E11 mol/cm3)Half-Life = 3. 720 HrsFraction sorbed to airborne particulates (phi): 3. 45E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 181. 1Log Koc: 2. 258 Aqueous Base/Acid-Catalyzed Hydrolysis (25 deg C) [HYDROWIN v1. 67]: Total Kb for pH > 8 at 25 deg C : 2. 069E-003 L/mol-secKb Half-Life at pH 8: 10. 614 years Kb Half-Life at pH 7: 106. 143 years Bioaccumulation Estimates from Log Kow (BCFWIN v2. 17): Log BCF from regression-based method = 0. 195 (BCF = 1. 566)log Kow used: 1. 16 (estimated)Volatilization from Water: Henry LC: 3. 86E-008 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 2. 042E+004 hours (850. 9 days)Half-Life from Model Lake : 2. 229E+005 hours (9287 days)Removal In Wastewater Treatment: Total removal: 1. 91 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 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. 111 1. 81 1000 Water 45. 1 900 1000 Soil 54. 7 1. 8e+003 1000 Sediment 0. 099 8. 1e+003 0 Persistence Time: 693 hr

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