2-carbomethoxy-8-methyl-8-azabicyclo[3.2.1]oct-2-ene c10h15no2 structure

Contents

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	162. 9±3. 0

Volume 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_37943

9,

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′-

furanoylecgoni

ne methyl

ester-isolation

and mass

spectral

characterizatio

n 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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