2-isocyanato-2-methylpropane c5h9no structure

Contents

- Safety:

Molecular Formula	C_5H_9NO
Average mass	99. 131 Da
Density	0. 8±0. 1 g/cm ^{3}
Boiling Point	85. 5±0. 0 °C at 760 mmHg
Flash Point	-4. 4±0. 0 °C
Molar Refractivity	29. 5±0. 5 cm ^{3}
Polarizability	11. 7±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	26. 1±7. 0 dyne/cm
Molar Volume	117. 3±7. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs
- Predicted – EPISuite

- Predicted – ChemAxon
- Predicted – Mcule
- Experimental Physico-chemical Properties

Experimental Melting Point:

85. 5 °CJean-Claude

Bradley Open Melting

Point Dataset22893

Experimental Boiling Point:

85-86 °CMatrix

Scientific

85-86 °CAlfa

AesarL13371

85-86 °CMatrix

Scientific080122

85-86

°CSynQuest62455,

4149-1-X0

85 °CBiosynthW-

107973

85-86 °C

(Literature)LabNetwork

LN00115283

- **Experimental Flash Point:**

  -4 °CAlfa Aesar

  -4 °CBiosynthW-107973

  -4 °F (-20 °C)Alfa

  AesarL13371

  -4 °CSynQuest62455, 4149-

  1-X0

  24

  °CLabNetworkLN00115283

- **Experimental Gravity:**

  0. 868 g/mLBiosynthW-

  107973

  0. 868 g/mLAlfa AesarL13371

  0. 868 g/mLMatrix

  Scientific080122

  0. 868 g/mLSynQuest4149-1-

  X0

  -4 g/mLBiosynthW-107973

- **Experimental Refraction Index:**

  1. 386Alfa AesarL13371

  1. 39SynQuest62455,

  4149-1-X0

- Miscellaneous

- **Safety:**

  11-22-26-36/37/38-

  42Alfa AesarL13371

  23-26-28-36/37-45Alfa

  AesarL13371

  6. 1Alfa AesarL13371

  DangerAlfa

  AesarL13371

  DangerBiosynthW-

  107973

  FLAMMABLE / HIGHLY

  TOXICAlfa AesarL13371

  GHS02; GHS05; GHS06;

  GHS08BiosynthW-

107973

H225; H302; H314;

H317; H330; H334;

H335BiosynthW-

107973

H225-H330-H334-

H302-H315-H319-

H335Alfa AesarL13371

IRRITANTMatrix

Scientific080122

P210; P260; P280;

P284;

P305+P351+P338;

P310BiosynthW-

107973

P210-

P303+P361+P353-

P304+P340-

P305+P351+P338-

P320-P330-P405-

P501aAlfa AesarL13371

Very

	Toxic/Flammable/Corro sive/Lachrymatory/Mois ture Sensitive/Store under Argon/Keep ColdSynQuest4149-1-X0, 62455

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

Density:	0. 8±0. 1 g/cm ^{3}
Boiling Point:	85. 5±0. 0 °C at 760 mmHg
Vapour Pressure:	69. 2±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	32. 6±3. 0 kJ/mol
Flash Point:	-4. 4±0. 0 °C
Index of Refraction:	1. 417
Molar Refractivity:	29. 5±0. 5 cm ^{3}
#H bond acceptors:	2
#H bond donors:	0
#Freely Rotating Bonds:	1

#Rule of 5 Violations:	0
ACD/LogP:	2. 06
ACD/LogD (pH 5. 5):	2. 02
ACD/BCF (pH 5. 5):	20. 32
ACD/KOC (pH 5. 5):	300. 47
ACD/LogD (pH 7. 4):	2. 02
ACD/BCF (pH 7. 4):	20. 32
ACD/KOC (pH 7. 4):	300. 47
Polar Surface Area:	29 Å ^{2}
Polarizability:	11. 7±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	26. 1±7. 0 dyne/cm
Molar Volume:	117. 3±7. 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. 15Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 92. 18 (Adapted Stein & Brown method)Melting Pt (deg C): -44. 75 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 13. 2 (Modified Grain method)MP (exp database): 85. 5 deg CSubcooled liquid VP: 50. 1 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): 1721log Kow used: 2. 15 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01

est) = 5061. 4 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: IsocyanatesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 17E-003 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 1. 000E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 15 (KowWin est)Log Kaw used: -1. 052 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 3. 202Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5164Biowin2 (Non-Linear Model) : 0. 4695Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7680 (weeks)Biowin4 (Primary Survey Model) : 3. 5513 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4861Biowin6 (MITI Non-Linear Model): 0. 5302Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2631Ready 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): 6. 68E+003 Pa (50. 1 mm Hg)Log Koa (Koawin est): 3. 202Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 49E-010 Octanol/air (Koa) model: 3. 91E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 62E-008 Mackay model : 3. 59E-008 Octanol/air (Koa) model: 3. 13E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 5018 E-12 cm3/molecule-secHalf-Life = 21. 314 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 61E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 178. 2Log Koc: 2. 251 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 = 0. 954 (BCF = 9. 002)log Kow used: 2. 15 (estimated)Volatilization from Water: Henry LC: 0. 00217 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 285 hoursHalf-Life from Model Lake : 97. 5 hours (4. 062 days)Removal In Wastewater Treatment: Total removal: 47. 60 percentTotal biodegradation: 0. 06 percentTotal sludge adsorption: 1. 51 percentTotal to Air: 46. 03 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 35. 7 511 1000 Water 35. 8 360 1000 Soil 28. 4 720 1000 Sediment 0. 15 3. 24e+003 0 Persistence Time: 186 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop