

# [2-isocyanato-2-methylpropane c5h9no structure](https://assignbuster.com/2-isocyanato-2-methylpropane-c5h9no-structure/)

Contents

* Safety:

|  |  |
| --- | --- |
| Molecular Formula  | C 5 H 9 NO  |
| 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)LabNetworkLN00115283  |

## 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/Corrosive/Lachrymatory/Moisture Sensitive/Store under Argon/Keep ColdSynQuest4149-1-X0, 62455  |

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

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| --- | --- |
| 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  |

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| 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

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