

# [M-cyanoanisole c8h7no structure](https://assignbuster.com/m-cyanoanisole-c8h7no-structure/)

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* Retention Index (Kovats):

|  |  |
| --- | --- |
| Molecular Formula  | C 8 H 7 NO  |
| Average mass  | 133. 147 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 233. 2±0. 0 °C at 760 mmHg  |
| Flash Point  | 105. 0±0. 0 °C  |
| Molar Refractivity  | 37. 7±0. 4 cm 3  |
| Polarizability  | 14. 9±0. 5 10 -24 cm 3  |
| Surface Tension  | 41. 8±5. 0 dyne/cm  |
| Molar Volume  | 122. 6±5. 0 cm 3  |

* Experimental data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* Experimental Physico-chemical Properties

## Experimental Melting Point:

|  |
| --- |
| 22-24 °CAlfa Aesar  |
| 23 °CJean-Claude Bradley Open Melting Point Dataset4060  |
| 22-24 °CAlfa AesarB24171  |
| 20-22 °CLabNetworkLN00183782  |
| 20-22 °CIndofine[CS-642]  |

## Experimental Boiling Point:

|  |
| --- |
| 110-111 deg C / 12 mm (258. 8631-260. 2162 °C / 760 mmHg)Alfa Aesar  |
| 110-111 °C / 12 mm (258. 8631-260. 2162 °C / 760 mmHg)Alfa AesarB24171  |
| 111-112 °C / 13 mmHg (257. 4099-258. 7562 °C / 760 mmHg)SynQuest57603, 4637-1-W1  |
| 111-112 °C / 13 mm (257. 4099-258. 7562 °C / 760 mmHg)Oakwood[035585]  |
| 111-112 °C / 13 mm (257. 4099-258. 7562 °C / 760 mmHg)LabNetworkLN00183782  |

## Experimental Flash Point:

|  |
| --- |
| 105 °CAlfa Aesar  |
| 105 °CAlfa Aesar  |
| 105 °F (40. 5556 °C)Alfa AesarB24171  |
| 105 °COakwood[035585]  |
| 105 °CLabNetworkLN00183782  |

## Experimental Gravity:

|  |
| --- |
| 1. 089 g/mLAlfa AesarB24171  |
| 1. 089 g/mLOakwood[035585]  |
| 1. 089 g/mLFluorochem  |
| 1. 089 g/lFluorochem035585  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 5402Alfa AesarB24171  |

* Miscellaneous

## Appearance:

|  |
| --- |
| Not AvailableNovochemy[NC-20570]  |

## Safety:

|  |
| --- |
| 20/21/22Novochemy[NC-20570]  |
| 20/21/22-36/38Alfa AesarB24171  |
| 20/21/36/37/39Novochemy[NC-20570]  |
| 26-36/37Alfa AesarB24171  |
| 6. 1Alfa AesarB24171  |
| DANGER: POISON, causes cyanosis; skin, eye, lung irritationAlfa AesarB24171  |
| GHS07; GHS09Novochemy[NC-20570]  |
| H302-H312-H332-H315-H319Alfa AesarB24171  |
| H332; H403Novochemy[NC-20570]  |
| IRRITANTMatrix Scientific084460  |
| IrritantSynQuest4637-1-W1, 57603  |
| P102; P210; P262; P270; P302+P352; P308+P313Novochemy[NC-20570]  |
| P261-P280-P305+P351+P338-P304+P340-P362-P501aAlfa AesarB24171  |
| R52/53Novochemy[NC-20570]  |
| WarningAlfa AesarB24171  |
| WarningNovochemy[NC-20570]  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1147 (estimated with error: 89)NIST Spectramainlib\_118642, replib\_117903  |

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

|  |  |
| --- | --- |
| Density:  | 1. 1±0. 1 g/cm 3  |
| Boiling Point:  | 233. 2±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 1±0. 4 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 47. 0±3. 0 kJ/mol  |
| Flash Point:  | 105. 0±0. 0 °C  |
| Index of Refraction:  | 1. 527  |
| Molar Refractivity:  | 37. 7±0. 4 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 2  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 1. 45  |
| ACD/LogD (pH 5. 5):  | 1. 71  |
| ACD/BCF (pH 5. 5):  | 11. 64  |
| ACD/KOC (pH 5. 5):  | 201. 66  |
| ACD/LogD (pH 7. 4):  | 1. 71  |
| ACD/BCF (pH 7. 4):  | 11. 64  |
| ACD/KOC (pH 7. 4):  | 201. 66  |
| Polar Surface Area:  | 33 Å 2  |
| Polarizability:  | 14. 9±0. 5 10 -24 cm 3  |
| Surface Tension:  | 41. 8±5. 0 dyne/cm  |
| Molar Volume:  | 122. 6±5. 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. 62Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 230. 92 (Adapted Stein & Brown method)Melting Pt (deg C): 27. 05 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0675 (Modified Grain method)Subcooled liquid VP: 0. 0704 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): 2003log Kow used: 1. 62 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 317. 27 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 3. 08E-006 atm-m3/moleGroup Method: 3. 62E-005 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 5. 904E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 62 (KowWin est)Log Kaw used: -3. 900 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 5. 520Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 1. 1231Biowin2 (Non-Linear Model) : 0. 9997Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7644 (weeks )Biowin4 (Primary Survey Model) : 3. 6676 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6162Biowin6 (MITI Non-Linear Model): 0. 6766Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 5528Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 9. 39 Pa (0. 0704 mm Hg)Log Koa (Koawin est ): 5. 520Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 2E-007 Octanol/air (Koa) model: 8. 13E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 15E-005 Mackay model : 2. 56E-005 Octanol/air (Koa) model: 6. 5E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 3. 6445 E-12 cm3/molecule-secHalf-Life = 2. 935 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 35. 218 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 1. 86E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 69. 86Log Koc: 1. 844 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. 548 (BCF = 3. 533)log Kow used: 1. 62 (estimated)Volatilization from Water: Henry LC: 3. 62E-005 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 19. 84 hoursHalf-Life from Model Lake : 313. 2 hours (13. 05 days)Removal In Wastewater Treatment: Total removal: 3. 91 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 89 percentTotal to Air: 1. 93 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 5. 9 70. 4 1000 Water 35. 6 360 1000 Soil 58. 4 720 1000 Sediment 0. 0907 3. 24e+003 0 Persistence Time: 360 hr

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