M-cyanoanisole c8h7no structure

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Molecular Formula	C_8H_7NO
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	37. 7±0. 4 cm ^{3}

Refractivity	
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 °CLabNetworkLN00183

782

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[03558

5]

111-112 °C / 13 mm

(257. 4099-258. 7562

°C / 760

mmHg)LabNetworkLN0

0183782

- **Experimental Flash Point:**

105 °CAlfa Aesar

105 °CAlfa Aesar

105 °F (40. 5556

°C)Alfa AesarB24171

105

°COakwood[035585]

105

°CLabNetworkLN00183

782

- **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[N

    C-20570]

    20/21/22-36/38Alfa

    AesarB24171

    20/21/36/37/39Novoch

    emy[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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- 1-Click Scaffold Hop