

# [3-cyanopyridine c6h4n2 structure](https://assignbuster.com/3-cyanopyridine-c6h4n2-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 6 H 4 N 2  |
| Average mass  | 104. 109 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 203. 0±13. 0 °C at 760 mmHg  |
| Flash Point  | 84. 4±0. 0 °C  |
| Molar Refractivity  | 29. 1±0. 4 cm 3  |
| Polarizability  | 11. 5±0. 5 10 -24 cm 3  |
| Surface Tension  | 51. 4±5. 0 dyne/cm  |
| Molar Volume  | 92. 8±5. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| 50 °CTCIC0456  |
| 48-51 °CAlfa Aesar  |
| 50 °COxford University Chemical Safety Data (No longer updated)More details  |
| 48-51 °CMerck Millipore1397, 802658  |
| 51 °CJean-Claude Bradley Open Melting Point Dataset22517  |
| 50 °CJean-Claude Bradley Open Melting Point Dataset16000, 3872  |
| 48-51 °CAlfa AesarA14850  |
| 48-52 °CLabNetworkLN00008274  |

## Experimental Boiling Point:

|  |
| --- |
| 206-208 °CAlfa Aesar  |
| 201 °COxford University Chemical Safety Data (No longer updated)More details  |
| 206-208 °CAlfa AesarA14850  |
| 201 °CLabNetworkLN00008274  |

## Experimental LogP:

|  |
| --- |
| 0. 503Vitas-MSTK046164  |

## Experimental Flash Point:

|  |
| --- |
| 84 °CAlfa Aesar  |
| 84 °COxford University Chemical Safety Data (No longer updated)More details  |
| 84 °CAlfa Aesar  |
| 84 °F (28. 8889 °C)Alfa AesarA14850  |
| 184 °CLabNetworkLN00008274  |

## Experimental Gravity:

|  |
| --- |
| 1. 16 g/mLAlfa AesarA14850  |
| 1. 159 g/mLFluorochem  |
| 1. 159 g/lFluorochem234028  |

* Predicted Physico-chemical Properties

## Predicted Melting Point:

|  |
| --- |
| 50 °CTCI  |
| 50 °CTCIC0456  |

* Miscellaneous

## Appearance:

|  |
| --- |
| White SolidNovochemy[NC-31305]  |
| white to beige solidOxford University Chemical Safety Data (No longer updated)More details  |

## Stability:

|  |
| --- |
| Incompatible with strong oxidizing agents, strong reducing agents, strong acids, strong bases. Oxford University Chemical Safety Data (No longer updated)More details  |

## Toxicity:

|  |
| --- |
| ORL-RAT LD50 1185 mg kg-1Oxford University Chemical Safety Data (No longer updated)More details  |

## Safety:

|  |
| --- |
| 20/21/36/37/39Novochemy[NC-31305]  |
| 22-36/37/38Alfa AesarA14850  |
| 26-36/37Alfa AesarA14850  |
| 36/37/38Novochemy[NC-31305]  |
| GHS07BiosynthW-108955  |
| GHS07; GHS09Novochemy[NC-31305]  |
| H302; H315; H319; H335BiosynthW-108955  |
| H302-H315-H319-H335Alfa AesarA14850  |
| H332; H403Novochemy[NC-31305]  |
| P261; P305+P351+P338BiosynthW-108955  |
| P280h-P305+P351+P338Alfa AesarA14850  |
| P305+P351+P338; P376; P270Novochemy[NC-31305]  |
| R52/53Novochemy[NC-31305]  |
| Safety glasses, adequate ventilation. Oxford University Chemical Safety Data (No longer updated)More details  |
| WarningAlfa AesarA14850  |
| WarningBiosynthW-108955  |
| WarningNovochemy[NC-31305]  |
| WARNING: Irritates skin and eyes, harmful if swallowedAlfa AesarA14850  |
| XnAbblis ChemicalsAB1001139  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 952 (estimated with error: 83)NIST Spectramainlib\_230614, replib\_135454, replib\_155088  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 964. 9 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 32 mm; Column length: 25 m; Column type: Capillary; Heat rate: 20 K/min; Start T: 50 C; End T: 250 C; Start time: 1 min; CAS no: 100549; Active phase: HP-1; Carrier gas: He; Data type: Normal alkane RI; Authors: Katritzky, A. R.; Ignatchenko, E. S.; Barcock, R. A.; Lobanov, V. S.; Karelson, M., Prediction of gas chromatographic retention times and response factors using a general quantitative structure — property relationship treatment, Anal. Chem., 66, 1994, 1799-1807.)NIST Spectranist ri  |
| 1012 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 30 C; End T: 260 C; End time: 28 min; Start time: 2 min; CAS no: 100549; Active phase: HP-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Leffingwell, J. C.; Alford, E. D., Volatile constituents of Perique tobacco, Electron. J. Environ. Agric. Food Chem., 4(2), 2005, 899-915.)NIST Spectranist ri  |
| 1877. 5 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 50 C; End T: 240 C; Start time: 2 min; CAS no: 100549; Active phase: Supelcowax-10; Carrier gas: He; Phase thickness: 0. 32 um; Data type: Normal alkane RI; Authors: Barrio, M. E.; Lliberia, J. Ll.; Comellas, L.; Broto-Puig, F., Pyrolysis-gas chromatography applied to the study of organic matter evolution in sewage sludge-amended soils using nitrogen-phosphorus, flame ionization and mass spectrometric detection, J. Chromatogr. A, 719, 1996, 131-139.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 1007 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 32 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 K/min; Start T: 60 C; End T: 280 C; End time: 3 min; Start time: 10 min; CAS no: 100549; Active phase: DB-5; Carrier gas: He; Data type: Linear RI; Authors: Premecz, J. E.; Ford, M. E., Gas chromatographic separation of substituted pyridines, J. Chromatogr., 388, 1987, 23-35.)NIST Spectranist ri  |
| 1875 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column diameter: 0. 25 mm; Column length: 60 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 230 C; End time: 60 min; CAS no: 100549; Active phase: DB-Wax; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Shimoda, M.; Shiratsuchi, H.; Nakada, Y.; Wu, Y.; Osajima, Y., Identification and sensory characterization of volatile flavor compounds in sesame seed oil, J. Agric. Food Chem., 44, 1996, 3909-3912.)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:  | 203. 0±13. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 3±0. 4 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 43. 9±3. 0 kJ/mol  |
| Flash Point:  | 84. 4±0. 0 °C  |
| Index of Refraction:  | 1. 540  |
| Molar Refractivity:  | 29. 1±0. 4 cm 3  |
| #H bond acceptors:  | 2  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 1  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 0. 50  |
| ACD/LogD (pH 5. 5):  | 0. 52  |
| ACD/BCF (pH 5. 5):  | 1. 48  |
| ACD/KOC (pH 5. 5):  | 45. 99  |
| ACD/LogD (pH 7. 4):  | 0. 52  |
| ACD/BCF (pH 7. 4):  | 1. 48  |
| ACD/KOC (pH 7. 4):  | 45. 99  |
| Polar Surface Area:  | 37 Å 2  |
| Polarizability:  | 11. 5±0. 5 10 -24 cm 3  |
| Surface Tension:  | 51. 4±5. 0 dyne/cm  |
| Molar Volume:  | 92. 8±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) = 0. 35Log Kow (Exper. database match) = 0. 36Exper. Ref: Sangster (1994)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 200. 84 (Adapted Stein & Brown method)Melting Pt (deg C): 25. 39 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 135 (Modified Grain method)MP (exp database): 51 deg CBP (exp database): 206. 9 deg CVP (exp database): 2. 96E-01 mm Hg at 25 deg CSubcooled liquid VP: 0. 535 mm Hg (25 deg C, exp database VP )Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 3. 042e+004log Kow used: 0. 36 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 96246 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 6. 81E-008 atm-m3/moleGroup Method: 4. 99E-008 atm-m3/moleExper Database: 2. 74E-07 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 6. 079E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 0. 36 (exp database)Log Kaw used: -4. 951 (exp database)Log Koa (KOAWIN v1. 10 estimate): 5. 311Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8504Biowin2 (Non-Linear Model) : 0. 9894Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 6725 (weeks-months)Biowin4 (Primary Survey Model) : 3. 6136 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4734Biowin6 (MITI Non-Linear Model): 0. 4439Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 0954Ready 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): 71. 3 Pa (0. 535 mm Hg)Log Koa (Koawin est ): 5. 311Kp (particle/gas partition coef. (m3/ug)): Mackay model : 4. 21E-008 Octanol/air (Koa) model: 5. 02E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 52E-006 Mackay model : 3. 36E-006 Octanol/air (Koa) model: 4. 02E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 0. 0653 E-12 cm3/molecule-secHalf-Life = 163. 720 Days (12-hr day; 1. 5E6 OH/cm3)Ozone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 44E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 98. 14Log Koc: 1. 992 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. 500 (BCF = 3. 162)log Kow used: 0. 36 (expkow database)Volatilization from Water: Henry LC: 2. 74E-007 atm-m3/mole (Henry experimental database)Half-Life from Model River: 2181 hours (90. 89 days)Half-Life from Model Lake : 2. 388E+004 hours (995. 1 days)Removal In Wastewater Treatment: Total removal: 1. 87 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 76 percentTotal to Air: 0. 02 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 2. 45 3. 93e+003 1000 Water 47. 8 900 1000 Soil 49. 6 1. 8e+003 1000 Sediment 0. 0939 8. 1e+003 0 Persistence Time: 777 hr

Click to predict properties on the Chemicalize site

* 1-Click Docking
* 1-Click Scaffold Hop