3-cyanopyridine c6h4n2 structure

ASSIGN BUSTER

Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_4N_2$
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      50 °COxford University Chemical Safety Data (No longer updated)More details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

°CLabNetworkLN00008

274

- **Experimental Boiling Point:**

  206-208 °CAlfa Aesar

  201 °COxford

  University Chemical

  Safety Data (No longer

  updated)More details

  206-208 °CAlfa

  AesarA14850

  201

  °CLabNetworkLN00008

  274

- **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

°CLabNetworkLN00008

274

- **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:**

  20/21/36/37/39Novoch

  emy[NC-31305]

  22-36/37/38Alfa

  AesarA14850

  26-36/37Alfa

  AesarA14850

  36/37/38Novochemy[N

  C-31305]

  GHS07BiosynthW-

  108955

  GHS07;

  GHS09Novochemy[NC-

31305]

H302; H315; H319;
H335BiosynthW-
108955

H302-H315-H319-
H335Alfa AesarA14850

H332;
H403Novochemy[NC-
31305]

P261;
P305+P351+P338Biosy
nthW-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