3-methoxypyridin-2-amine c6h8n2o structure

Contents

- Safety:

Molecular Formula	$C_6H_8N_2O$
Average mass	124. 141 Da
Density	1. 1±0. 1 g/cm ^{3}
Boiling Point	235. 0±20. 0 °C at 760 mmHg
Flash Point	95. 9±21. 8 °C
Molar Refractivity	35. 3±0. 3 cm ^{3}
Polarizability	14. 0±0. 5 10^{-24} cm ^{3}
Surface Tension	46. 1±3. 0 dyne/cm
Molar Volume	108. 9±3. 0 cm ^{3}

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

      235 °CBiosynthW-

      204442
    - **Experimental Flash Point:**

      95. 92 °CBiosynthW-

      204442
    - **Experimental Gravity:**

      95. 92 g/mLBiosynthW-

      204442
- Predicted Physico-chemical Properties
    - **Predicted Melting Point:**

      76-78 °CEnamineEN300-

      60484
- Miscellaneous

- **Appearance:**

  Gray

  PowderNovochem

  y[NC-02615]

  gray

  solidNovochemy[N

  C-02615]

- **Safety:**

  20/21/36/37/39No

  vochemy[NC-

  02615]

  36/37/38Novoche

  my[NC-02615]

  GHS07;

  GHS09Novochemy

  [NC-02615]

  H304;

  H403Novochemy[

  NC-02615]

  IRRITANTMatrix

  Scientific072687

Irritant/Keep

Cold/Store under

ArgonSynQuest4H

30-1-01, 57116

P332+P313;

P305+P351+P338

Novochemy[NC-

02615]

R22Novochemy[N

C-02615]

R22,

R36/37/38SynQue

st4H30-1-01

R36/37/38SynQue

st4H30-1-01,

57116

S13, S23, S24/25,

S26, S36/37/39,

S45SynQuest4H30

-1-01, 57116

S22, S24/25, S26,

S36/37/39,

S45SynQuest4H30

-1-01

WarningNovoche

my[NC-02615]

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

Density:	1. 1±0. 1 g/cm ^{3}
Boiling Point:	235. 0±20. 0 °C at 760 mmHg
Vapour Pressure:	0. 1±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	47. 2±3. 0 kJ/mol
Flash Point:	95. 9±21. 8 °C
Index of Refraction:	1. 561
Molar Refractivity:	35. 3±0. 3 cm ^{3}
#H bond acceptors:	3
#H bond donors:	2
#Freely Rotating Bonds:	1
#Rule of 5 Violations:	0

ACD/LogP:	1. 21
ACD/LogD (pH 5. 5):	-1. 32
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-0. 01
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	7. 71
Polar Surface Area:	48 Å ^{2}
Polarizability:	14. 0±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	46. 1±3. 0 dyne/cm
Molar Volume:	108. 9±3. 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. 61Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 232. 86 (Adapted Stein & Brown method)Melting Pt (deg C): 48. 27 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0391 (Modified Grain method)Subcooled liquid VP: 0. 0638 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): 2. 916e+004log Kow used: 0. 61 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 1e+006 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aromatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 47E-010 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 2. 190E-007 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg

C) [KOAWIN v1. 10]: Log Kow used: 0. 61 (KowWin est)Log Kaw used: -8. 221 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 8. 831Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 4320Biowin2 (Non-Linear Model) : 0. 4873Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 5176 (weeks-months)Biowin4 (Primary Survey Model) : 3. 6186 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3719Biowin6 (MITI Non-Linear Model): 0. 2608Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 1. 0115Ready 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): 8. 51 Pa (0. 0638 mm Hg)Log Koa (Koawin est): 8. 831Kp (particle/gas partition coef. (m3/ug)): Mackay model : 3. 53E-007 Octanol/air (Koa) model: 0. 000166 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 27E-005 Mackay model : 2. 82E-005 Octanol/air (Koa) model: 0. 0131 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 18. 4989 E-12 cm3/molecule-secHalf-Life = 0. 578 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 6. 938 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 05E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 32. 54Log Koc: 1. 512 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. 61 (estimated)Volatilization from Water: Henry LC: 1. 47E-010 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 4. 438E+006 hours (1. 849E+005 days)Half-Life from Model Lake : 4. 841E+007 hours (2. 017E+006 days)Removal In Wastewater Treatment: Total removal: 1. 86 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 77 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 00199 13. 9 1000 Water 43. 8 900 1000 Soil 56. 1 1. 8e+003 1000 Sediment 0. 0876 8. 1e+003 0 Persistence Time: 1. 01e+003 hr

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- 1-Click Scaffold Hop