

# [3-methoxypyridin-2-amine c6h8n2o structure](https://assignbuster.com/3-methoxypyridin-2-amine-c6h8n2o-structure/)

Contents

* Safety:

|  |  |
| --- | --- |
| Molecular Formula | C 6 H 8 N 2 O |
| 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:

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| --- |
| Gray PowderNovochemy[NC-02615] |
| gray solidNovochemy[NC-02615] |

## Safety:

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| --- |
| 20/21/36/37/39Novochemy[NC-02615] |
| 36/37/38Novochemy[NC-02615] |
| GHS07; GHS09Novochemy[NC-02615] |
| H304; H403Novochemy[NC-02615] |
| IRRITANTMatrix Scientific072687 |
| Irritant/Keep Cold/Store under ArgonSynQuest4H30-1-01, 57116 |
| P332+P313; P305+P351+P338Novochemy[NC-02615] |
| R22Novochemy[NC-02615] |
| R22, R36/37/38SynQuest4H30-1-01 |
| R36/37/38SynQuest4H30-1-01, 57116 |
| S13, S23, S24/25, S26, S36/37/39, S45SynQuest4H30-1-01, 57116 |
| S22, S24/25, S26, S36/37/39, S45SynQuest4H30-1-01 |
| WarningNovochemy[NC-02615] |

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

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| --- | --- |
| 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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