

# [6-methylquinoline c10h9n structure](https://assignbuster.com/6-methylquinoline-c10h9n-structure/)

Contents

* Retention Index (Linear):

|  |  |
| --- | --- |
| Molecular Formula  | C 10 H 9 N  |
| Average mass  | 143. 185 Da  |
| Density  | 1. 1±0. 1 g/cm 3  |
| Boiling Point  | 258. 6±0. 0 °C at 760 mmHg  |
| Flash Point  | 104. 4±11. 3 °C  |
| Molar Refractivity  | 47. 0±0. 3 cm 3  |
| Polarizability  | 18. 6±0. 5 10 -24 cm 3  |
| Surface Tension  | 44. 1±3. 0 dyne/cm  |
| Molar Volume  | 133. 0±3. 0 cm 3  |

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

## Experimental Melting Point:

|  |
| --- |
| -22 °CAlfa Aesar  |
| -22 °CJean-Claude Bradley Open Melting Point Dataset20934, 6174  |
| -22 °CAlfa AesarB21892  |
| -22 °CLabNetworkLN00132358  |
| -22 °CFooDBFDB011115  |

## Experimental Boiling Point:

|  |
| --- |
| 257-259 °CAlfa Aesar  |
| 259 °CFood and Agriculture Organization of the United Nations6-Methylquinoline  |
| 257-259 °CAlfa AesarB21892  |
| 259 °CLabNetworkLN00132358  |
| 100 °C / 181 mmHg (151. 2241 °C / 760 mmHg)FooDBFDB011115  |

## Experimental Flash Point:

|  |
| --- |
| 110 °CAlfa Aesar  |
| 110 °CAlfa Aesar  |
| 110 °F (43. 3333 °C)Alfa AesarB21892  |
| 230 °CLabNetworkLN00132358  |

## Experimental Gravity:

|  |
| --- |
| 1. 066 g/mLAlfa AesarB21892  |

## Experimental Refraction Index:

|  |
| --- |
| 1. 614Alfa AesarB21892  |
| 1. 611-1. 617Food and Agriculture Organization of the United Nations6-Methylquinoline  |

* Miscellaneous

## Appearance:

|  |
| --- |
| Colourless oily liquid; Pungent heavy quinoline-like odourFood and Agriculture Organization of the United Nations6-Methylquinoline  |
| Not AvailableNovochemy[NC-01043]  |

## Safety:

|  |
| --- |
| 20/21/22Novochemy[NC-01043]  |
| 20/21/36/37/39Novochemy[NC-01043]  |
| 22-36/38-68Alfa AesarB21892  |
| 26-36/37Alfa AesarB21892  |
| GHS07; GHS09Novochemy[NC-01043]  |
| H304; H403Novochemy[NC-01043]  |
| H341-H302-H315-H319Alfa AesarB21892  |
| P280-P281-P305+P351+P338-P362-P405-P501aAlfa AesarB21892  |
| P332+P313; P305+P351+P338Novochemy[NC-01043]  |
| WarningAlfa AesarB21892  |
| WarningNovochemy[NC-01043]  |
| WARNING: Irritates skin and eyes, harmful if swallowedAlfa AesarB21892  |
| XnNovochemy[NC-01043]  |

* Gas Chromatography

## Retention Index (Kovats):

|  |
| --- |
| 1338 (estimated with error: 83)NIST Spectramainlib\_291569, replib\_3975, replib\_228760  |
| 1343 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: Capillary; Start T: 140 C; CAS no: 91623; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Berlizov, Yu. S.; Nabivach, V. M.; Mitrikov, V. P., Capillary gas chromatography of alkylquinolines, Zh. Anal. Khim., 62(6), 1987, 1119-1124., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 140 C; CAS no: 91623; Active phase: OV-101; Carrier gas: He; Data type: Kovats RI; Authors: Dmitrikov, V. P.; Nabivach, V. M., Physico-chemical regularities of quinoline bases retention in gas chromatography, Coke Chem. (Engl. Transl.), , 1995, 27-34.)NIST Spectranist ri  |
| 1358 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 22 mm; Column length: 50 m; Column type: Capillary; Start T: 160 C; CAS no: 91623; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Berlizov, Yu. S.; Nabivach, V. M.; Mitrikov, V. P., Capillary gas chromatography of alkylquinolines, Zh. Anal. Khim., 62(6), 1987, 1119-1124., Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Capillary; Start T: 160 C; CAS no: 91623; Active phase: OV-101; Carrier gas: He; Data type: Kovats RI; Authors: Dmitrikov, V. P.; Nabivach, V. M., Physico-chemical regularities of quinoline bases retention in gas chromatography, Coke Chem. (Engl. Transl.), , 1995, 27-34.)NIST Spectranist ri  |
| 1335 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column diameter: 0. 23 mm; Column length: 20 m; Column type: Capillary; Start T: 150 C; CAS no: 91623; Active phase: OV-101; Carrier gas: N2; Data type: Kovats RI; Authors: Morishita, F.; Morimoto, S.; Kojima, T., Prediction of molecular structures of aza-arenes by retention indices and fluorescence spectra, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 688-692.)NIST Spectranist ri  |
| 1995 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Start T: 140 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Berlizov, Yu. S.; Nabivach, V. M.; Mitrikov, V. P., Capillary gas chromatography of alkylquinolines, Zh. Anal. Khim., 62(6), 1987, 1119-1124., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Start T: 140 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Buryan, P.; Macak, J.; Triska, J.; Vodicka, L.; Berlizov, Yu. S.; Dmitrikov, V. P.; Nabivach, V. M., Kovats retention indices of alkylquinolines on capillary columns, J. Chromatogr., 391, 1987, 89-96., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 140 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: He; Data type: Kovats RI; Authors: Dmitrikov, V. P.; Nabivach, V. M., Physico-chemical regularities of quinoline bases retention in gas chromatography, Coke Chem. (Engl. Transl.), , 1995, 27-34.)NIST Spectranist ri  |
| 2020 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Start T: 160 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Berlizov, Yu. S.; Nabivach, V. M.; Mitrikov, V. P., Capillary gas chromatography of alkylquinolines, Zh. Anal. Khim., 62(6), 1987, 1119-1124., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Start T: 160 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Buryan, P.; Macak, J.; Triska, J.; Vodicka, L.; Berlizov, Yu. S.; Dmitrikov, V. P.; Nabivach, V. M., Kovats retention indices of alkylquinolines on capillary columns, J. Chromatogr., 391, 1987, 89-96., Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 160 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: He; Data type: Kovats RI; Authors: Dmitrikov, V. P.; Nabivach, V. M., Physico-chemical regularities of quinoline bases retention in gas chromatography, Coke Chem. (Engl. Transl.), , 1995, 27-34.)NIST Spectranist ri  |
| 2016 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column diameter: 0. 23 mm; Column length: 20 m; Column type: Capillary; Start T: 150 C; CAS no: 91623; Active phase: PEG-20M; Carrier gas: N2; Data type: Kovats RI; Authors: Morishita, F.; Morimoto, S.; Kojima, T., Prediction of molecular structures of aza-arenes by retention indices and fluorescence spectra, J. Hi. Res. Chromatogr. & Chromatogr. Comm., 9, 1986, 688-692.)NIST Spectranist ri  |

## Retention Index (Lee):

|  |
| --- |
| 230. 75 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column diameter: 0. 22 mm; Column length: 25 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 50 C; End T: 300 C; CAS no: 91623; Active phase: OV-101; Carrier gas: H2; Data type: Lee RI; Authors: Blanco, C. G.; Blanco, J.; Bermejo, J.; Guillen, M. D., Capillary gas chromatography of some polycyclic aromatic compounds on several stationary phases, J. Chromatogr., 465, 1989, 378-385.)NIST Spectranist ri  |
| 229. 82 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 3 mm; Column length: 12 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 50 C; End T: 250 C; CAS no: 91623; Active phase: SE-52; Carrier gas: He; Phase thickness: 0. 34 um; Data type: Lee RI; Authors: Lee, M. L.; Vassilaros, D. L.; White, C. M.; Novotny, M., Retention Indices for Programmed-Temperature Capillary-Column Gas Chromatography of Polycyclic Aromatic Hydrocarbons, Anal. Chem., 51(6), 1979, 768-773.)NIST Spectranist ri  |

## Retention Index (Normal Alkane):

|  |
| --- |
| 1351. 3 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 25 m; Column type: Capillary; Description: 70 0C (1 min) ^ 10 0C/min -> 130 0C ^ 6 0C/min -> 260 0C (20 min); CAS no: 91623; Active phase: SE-52; Carrier gas: He; Phase thickness: 0. 17 um; Data type: Normal alkane RI; Authors: Onuska, F. I.; Terry, K. A., Identification and quantitative analysis of nigrogen-containing polycyclic aromatic hydrocarbons in sediments, J. Hi. Res. Chromatogr., 12, 1989, 362-367.)NIST Spectranist ri  |

## Retention Index (Linear):

|  |
| --- |
| 1321. 2 (Program type: Ramp; Column cl… (show more)ass: Standard non-polar; Column type: Capillary; Heat rate: 8 K/min; Start T: 35 C; End T: 300 C; CAS no: 91623; Active phase: OV-1; Data type: Linear RI; Authors: Gautzsch, R.; Zinn, P., Use of incremental models to estimate the retention indexes of aromatic compounds, Chromatographia, 43(3/4), 1996, 163-176.)NIST Spectranist ri  |
| 2062 (Program type: Ramp; Column cl… (show more)ass: Standard polar; Column length: 3. 05 m; Column type: Packed; Heat rate: 8 K/min; Start T: 40 C; End T: 200 C; End time: 60 min; Start time: 4 min; CAS no: 91623; Active phase: Carbowax 20M; Substrate: Supelcoport; Data type: Linear RI; Authors: Peng, C. T.; Yang, Z. C.; Ding, S. F., Prediction of rentention idexes. II. Structure-retention index relationship on polar columns, J. Chromatogr., 586, 1991, 85-112.)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:  | 258. 6±0. 0 °C at 760 mmHg  |
| Vapour Pressure:  | 0. 0±0. 5 mmHg at 25°C  |
| Enthalpy of Vaporization:  | 47. 6±3. 0 kJ/mol  |
| Flash Point:  | 104. 4±11. 3 °C  |
| Index of Refraction:  | 1. 625  |
| Molar Refractivity:  | 47. 0±0. 3 cm 3  |
| #H bond acceptors:  | 1  |
| #H bond donors:  | 0  |
| #Freely Rotating Bonds:  | 0  |
| #Rule of 5 Violations:  | 0  |

|  |  |
| --- | --- |
| ACD/LogP:  | 2. 54  |
| ACD/LogD (pH 5. 5):  | 2. 39  |
| ACD/BCF (pH 5. 5):  | 34. 99  |
| ACD/KOC (pH 5. 5):  | 394. 75  |
| ACD/LogD (pH 7. 4):  | 2. 57  |
| ACD/BCF (pH 7. 4):  | 52. 33  |
| ACD/KOC (pH 7. 4):  | 590. 33  |
| Polar Surface Area:  | 13 Å 2  |
| Polarizability:  | 18. 6±0. 5 10 -24 cm 3  |
| Surface Tension:  | 44. 1±3. 0 dyne/cm  |
| Molar Volume:  | 133. 0±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) = 2. 69Log Kow (Exper. database match) = 2. 57Exper. Ref: Hansch, C et al. (1995)Log Kow (Exper. database match) = 2. 47Exper. Ref: Hansch, C et al. (1995)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 257. 71 (Adapted Stein & Brown method)Melting Pt (deg C): 54. 65 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0134 (Modified Grain method)MP (exp database): 39 deg CBP (exp database): 257. 6 deg CVP (exp database): 8. 84E-03 mm Hg at 25 deg CSubcooled liquid VP: 0. 0122 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): 631. 1log Kow used: 2. 47 (expkow database)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 2367. 8 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 7. 60E-007 atm-m3/moleGroup Method: 1. 65E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 4. 000E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 2. 47 (exp database)Log Kaw used: -4. 508 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 6. 978Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 7340Biowin2 (Non-Linear Model) : 0. 8253Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8079 (weeks )Biowin4 (Primary Survey Model) : 3. 5726 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3769Biowin6 (MITI Non-Linear Model): 0. 3589Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 1083Ready 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): 1. 63 Pa (0. 0122 mm Hg)Log Koa (Koawin est ): 6. 978Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 84E-006 Octanol/air (Koa) model: 2. 33E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 6. 66E-005 Mackay model : 0. 000148 Octanol/air (Koa) model: 0. 000187 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 30. 4189 E-12 cm3/molecule-secHalf-Life = 0. 352 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 4. 219 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 000107 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2976Log Koc: 3. 474 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 = 1. 202 (BCF = 15. 92)log Kow used: 2. 47 (expkow database)Volatilization from Water: Henry LC: 1. 65E-006 atm-m3/mole (estimated by Group SAR Method)Half-Life from Model River: 425. 8 hours (17. 74 days)Half-Life from Model Lake : 4746 hours (197. 7 days)Removal In Wastewater Treatment: Total removal: 3. 10 percentTotal biodegradation: 0. 10 percentTotal sludge adsorption: 2. 91 percentTotal to Air: 0. 09 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 809 8. 44 1000 Water 27. 4 360 1000 Soil 71. 6 720 1000 Sediment 0. 182 3. 24e+003 0 Persistence Time: 447 hr

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* 1-Click Scaffold Hop