6-methylquinoline c10h9n structure

Contents

- Retention Index (Linear):

Molecular Formula	$C_{10}H_9N$
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 °CLabNetworkLN00132 358

    -22 °CFooDBFDB011115

  - **Experimental Boiling Point:**

    257-259 °CAlfa Aesar

    259 °CFood and Agriculture Organization of the

United Nations6-

Methylquinoline

257-259 °CAlfa

AesarB21892

259

°CLabNetworkLN00132

358

100 °C / 181 mmHg

(151. 2241 °C / 760

mmHg)FooDBFDB0111

15

- **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[N

  C-01043]

- **Safety:**

  20/21/22Novochemy[N

  C-01043]

  20/21/36/37/39Novoch

  emy[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+P338Novo

chemy[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

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop