Dicyclohexylamine c12h23n structure

Contents

Molecular Formula	$C_{12}H_{23}N$
Average mass	181. 318 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	256. 1±8. 0 °C at 760 mmHg
Flash Point	96. 1±0. 0 °C
Molar Refractivity	57. 1±0. 4 cm ^{3}
Polarizability	22. 6±0. 5 10^{-24} cm^3
Surface Tension	33. 2±5. 0 dyne/cm
Molar Volume	198. 3±5. 0 cm^3

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

- **Experimental Melting Point:**

  -2 °CAlfa Aesar

  -1 °COxford University Chemical Safety Data (No longer updated)More details

  -1 °CJean-Claude Bradley Open Melting Point Dataset15987

  -0. 1 °CJean-Claude Bradley Open Melting Point

Dataset20653

-2 °CJean-Claude Bradley Open Melting Point Dataset14297, 6814

-2 °CAlfa AesarA15671

-2 °COakwood0984 46

- **Experimental Boiling Point:**

256 °CAlfa Aesar

256 °COxford University Chemical Safety Data (No longer updated)More details

256 °CAlfa AesarA15671

255-257

°COakwood0984

46

- **Experimental Flash Point:**

99 °CAlfa Aesar

99 °COxford

University

Chemical Safety

Data (No longer

updated)More

details

99 °CAlfa Aesar

99 °F (37. 2222

°C)Alfa

AesarA15671

96

°COakwood0984

46

- **Experimental Gravity:**

20 g/mLMerck

Millipore1441

20 g/lMerck

Millipore1441,

802948

0. 913 g/mLAlfa

AesarA15671

0. 912

g/mLOakwood09

8446

- **Experimental Refraction Index:**

  1. 4842Alfa

  AesarA15671

- Miscellaneous

  - **Appearance:**

    colourless or

    light yellow

    liquidOxford

    University

    Chemical Safety

    Data (No longer

    updated)More

details

- **Stability:**

  Stable.

  Incompatible

  with strong

  acids, strong

  oxidizing agents.

  Oxford University

  Chemical Safety

  Data (No longer

  updated)More

  details

- **Toxicity:**

  ORL-RAT LD50

  373 mg kg-1,

  SCU-MUS LD50

  135 mg kg-

  1Oxford

  University

  Chemical Safety

  Data (No longer

  updated)More

  details

- **Safety:**

  1/2-26-36/37/39-

  45-60-61Alfa

  AesarA15671

  22-34-50/53Alfa

  AesarA15671

  26-36/37/39-45-

  60-61Alfa

  AesarA15671

  8Alfa

  AesarA15671

  DangerAlfa

  AesarA15671

  DANGER:

  CORROSIVE,

  burns skin and

  eyesAlfa

  AesarA15671

  H314-H400-

  H410-H302Alfa

  AesarA15671

P260-
P303+P361+P35
3-
P305+P351+P33
8-
P301+P330+P33
1-P405-
P501aAlfa
AesarA15671

Safety glasses,
adequate
ventilation.
Oxford University
Chemical Safety
Data (No longer
updated)More
details

- Gas Chromatography

- **Retention Index (Kovats):**

  1540 (estimated
  with error:
  83)NIST
  Spectramainlib_2
  90817,

replib_7528,

replib_228971

1431. 48

(Program type:

Isothermal; Col…

(show more)umn

class: Standard

non-polar;

Column

diameter: 0. 53

mm; Column

length: 30 m;

Column type:

Capillary; Start T:

170 C; CAS no:

101837; Active

phase: DB-1;

Carrier gas: He;

Phase thickness:

3 um; Data type:

Kovats RI;

Authors: Kuhn, E.

R., Selectivity vs.

polarity: the

fundamentals of

chromatographic

separation, J.

Sep. Sci., 24,

2001, 473-

476.)NIST

Spectranist ri

- **Retention Index (Normal Alkane):**

  1392 (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: 3 K/min;

  Start T: 80 C;

  End T: 260 C;

  CAS no: 101837;

  Active phase:

  Ultra-1; Carrier

  gas: He; Phase

thickness: 0. 25 um; Data type: Normal alkane RI; Authors: Okumura, T., retention indices of environmental chemicals on methyl silicone capillary column, Journal of Environmental Chemistry (Japan), 1(2), 1991, 333-358.)NIST Spectranist ri

1437 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T:

150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia , 6(7), 1973, 293-300.)NIST

Spectranist ri

1442 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated

open tubular columns for a series of central nervous system stimulating drugs, Chromatographia , 6(7), 1973, 293-300.)NIST Spectranist ri

1444 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Apieson L / KOH; Data type: Normal alkane RI; Authors: Caddy,

B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia , 6(7), 1973, 293-300.)NIST Spectranist ri

1663 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type:

Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia , 6(7), 1973, 293-300.)NIST

Spectranist ri

1673 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D., Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular

columns for a series of central nervous system stimulating drugs, Chromatographia, 6(7), 1973, 293-300.)NIST Spectranist ri

1683 (Program type: Isothermal; Col… (show more)umn class: Standard polar; Column type: Capillary; Start T: 150 C; CAS no: 101837; Active phase: Carbowax 20M / KOH; Data type: Normal alkane RI; Authors: Caddy, B.; Fish, F.; Scott, D.,

Chromatographic screening for drugs of abuse using capillary columds. II. Peak identification on support coated open tubular columns for a series of central nervous system stimulating drugs, Chromatographia , 6(7), 1973, 293-300.)NIST Spectranist ri

- **Retention Index (Linear):**

1408 (Program type: Complex; Column... (show more)class: Standard non-polar; Column diameter: 0. 22

mm; Column length: 12 m; Column type: Capillary; Description: 120C=> 8C/min=> 270C=> 25C/min=> 300C; CAS no: 101837; Active phase: BP-1; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Stowell, A.; Wilson, L. W., A simple approach to the interlaboratory transfer of drug retention indices determined by temperature programmed

capillary gas chromatography, J. Forensic Sci., 32(5), 1987, 1214-1220.)NIST Spectranist ri

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

Density:	0. 9±0. 1 g/cm ^{3}
Boiling Point:	256. 1±8. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 5 mmHg at 25°C
Enthalpy of Vaporization:	49. 4±3. 0 kJ/mol
Flash Point:	96. 1±0. 0 °C
Index of Refraction:	1. 488
Molar Refractivity:	57. 1±0. 4 cm ^{3}
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	2
#Rule of 5 Violations:	0

ACD/LogP:	3. 69
ACD/LogD (pH 5. 5):	0. 58
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 89
ACD/LogD (pH 7. 4):	0. 62
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	2. 11
Polar Surface Area:	12 Å ^{2}
Polarizability:	22. 6±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	33. 2±5. 0 dyne/cm
Molar Volume:	198. 3±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) = 4. 37Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 256. 50 (Adapted Stein & Brown method)Melting Pt (deg C): 27. 68 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 02 (Mean VP of Antoine & Grain methods)MP (exp database): -0. 1 deg CBP (exp database): 255. 8 deg CVP (exp database): 3. 38E-02 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 103. 1log Kow used: 4. 37 (estimated)no-melting pt equation usedWater Sol Estimate from

Fragments: Wat Sol (v1. 01 est) = 1896. 6 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 50E-005 atm-m3/moleGroup Method: IncompleteHenrys LC [VP/WSol estimate using EPI values]: 4. 628E-005 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 4. 37 (KowWin est)Log Kaw used: -2. 648 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 7. 018Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8151Biowin2 (Non-Linear Model) : 0. 8240Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 8229 (weeks)Biowin4 (Primary Survey Model) : 3. 6294 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4281Biowin6 (MITI Non-Linear Model): 0. 2917Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 1079Ready 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): 4. 51 Pa (0. 0338 mm Hg)Log Koa (Koawin est): 7. 018Kp (particle/gas partition coef. (m3/ug)): Mackay model : 6. 66E-007 Octanol/air (Koa) model: 2. 56E-006 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 2. 4E-005 Mackay model : 5. 33E-005 Octanol/air (Koa) model: 0. 000205 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 131. 7220 E-12 cm3/molecule-secHalf-Life = 0. 081 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 0. 974 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 3. 86E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 256. 3Log Koc: 2. 409 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 = 2. 662 (BCF = 459. 5)log Kow used: 4. 37 (estimated)Volatilization from Water: Henry LC: 5. 5E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 15. 71 hoursHalf-Life from Model Lake : 284. 3 hours (11. 84 days)Removal In Wastewater Treatment: Total removal: 50. 04 percentTotal biodegradation: 0. 46 percentTotal sludge adsorption: 48. 18 percentTotal to Air: 1. 40 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 219 1. 95 1000 Water 20. 6 360 1000 Soil 73. 3 720 1000 Sediment 5. 9 3. 24e+003 0 Persistence Time: 471 hr

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- 1-Click Scaffold Hop