1,2-dicyclohexylethane c14h26 structure

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\n[/toc]\n \n

Contents

Molecular Formula	$C_{14}H_{26}$
Average mass	194. 356 Da
Density	0. 9±0. 1 g/cm ^{3}
Boiling Point	272. 2±7. 0 °C at 760 mmHg
Flash Point	106. 7±11. 7 °C
Molar Refractivity	62. 7±0. 3 cm ^{3}
Polarizability	24. 8±0. 5 10^{-24}

	cm ^{3}
Surface Tension	31. 6±3. 0 dyne/cm
Molar Volume	226. 5±3. 0 cm ^{3}

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

    11. 5 °CJean-Claude

    Bradley Open Melting

    Point Dataset23962
  - **Experimental Boiling Point:**

    142-144 °C / 15 mm

    (293. 715-296. 3794

    °C / 760

    mmHg)LabNetworkL

    N01318628
- Gas Chromatography

- **Retention Index (Kovats):**

  1540 (estimated with error: 39)NIST Spectramainlib_34892

  1498 (Program type: Isothermal; Col… (show more)umn class: Standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 3321504; Active phase: SE-30; Data type: Kovats RI; Authors: Shlyakhov, A. F.; Anvaer, B. I.; Zolotareva, O. V.; Romina, N. N.; Novikova, N. V.; Koreshkova, R. I., On the possibility of group indentification of hydrocarbons by gas chromatography from temperature

coefficients of
retention indices, Zh.
Anal. Khim., 30,
1975, 788-792.)NIST
Spectranist ri

1529 (Program type:
Isothermal; Col...
(show more)umn
class: Standard non-
polar; Column type:
Packed; Start T: 200
C; CAS no: 3321504;
Active phase: SE-30;
Data type: Kovats RI;
Authors: Shlyakhov,
A. F.; Anvaer, B. I.;
Zolotareva, O. V.;
Romina, N. N.;
Novikova, N. V.;
Koreshkova, R. I., On
the possibility of
group indentification
of hydrocarbons by
gas chromatography
from temperature

coefficients of
retention indices, Zh.
Anal. Khim., 30,
1975, 788-792.)NIST
Spectranist ri

1490 (Program type:
Isothermal; Col…
(show more)umn
class: Standard non-
polar; Column type:
Packed; Start T: 130
C; CAS no: 3321504;
Active phase: Methyl
Silicone; Data type:
Kovats RI; Authors:
Antheaume, J.;
Guiochon, G.,
Application de la
chromatographie en
phase gazeuse a
l’etude de la
composition des
fractions moyennes
d’un brut petrolier,
Bull. Soc. Chim. Fr.,

2, 1965, 298-307.,

Program type:

Isothermal; Col…

(show more)umn

class: Standard non-

polar; Column type:

Packed; Start T: 130

C; CAS no: 3321504;

Active phase: SE-30;

Data type: Kovats RI;

Authors: Antheaume,

J.; Guiochon, G.,

Application de la

chromatographie en

phase gazeuse a

l’etude de la

composition des

fractions moyennes

d’un brut petrolier,

Bull. Soc. Chim. Fr.,

2, 1965, 298-

307.)NIST

Spectranist ri

1507 (Program type:

Isothermal; Col…

(show more)umn
class: Standard non-
polar; Column type:
Packed; Start T: 170
C; CAS no: 3321504;
Active phase: SE-30;
Data type: Kovats RI;
Authors: Antheaume,
J.; Guiochon, G.,
Application de la
chromatographie en
phase gazeuse a
l’etude de la
composition des
fractions moyennes
d’un brut petrolier,
Bull. Soc. Chim. Fr.,
2, 1965, 298-
307.)NIST
Spectranist ri

1515 (Program type:
Isothermal; Col…
(show more)umn
class: Standard non-
polar; Column type:

Packed; Start T: 184 C; CAS no: 3321504; Active phase: SE-30; Data type: Kovats RI; Authors: Antheaume, J.; Guiochon, G., Application de la chromatographie en phase gazeuse a l’etude de la composition des fractions moyennes d’un brut petrolier, Bull. Soc. Chim. Fr., 2, 1965, 298-307.)NIST Spectranist ri

1544 (Program type: Isothermal; Col… (show more)umn class: Semi-standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 3321504; Active

phase: Apiezon L;
Data type: Kovats RI;
Authors: Shlyakhov,
A. F.; Anvaer, B. I.;
Zolotareva, O. V.;
Romina, N. N.;
Novikova, N. V.;
Koreshkova, R. I., On
the possibility of
group indentification
of hydrocarbons by
gas chromatography
from temperature
coefficients of
retention indices, Zh.
Anal. Khim., 30,
1975, 788-792.)NIST
Spectranist ri

- **Retention Index (Linear):**

  1486. 9 (Program
  type: Ramp; Column
  cl… (show more)ass:
  Semi-standard non-
  polar; Column
  diameter: 0. 25 mm;

Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm;

Column length: 30 m; Column type: Capillary; Heat rate: 2 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer

Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spectranist ri

1495 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; Start time: 5 min; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed

retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; Start time: 5 min; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy,

K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)NIST Spectranist ri

1496. 3 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type:

Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., Program type: Ramp; Column cl... (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type:

Capillary; Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York,

2003, 147-193.)NIST Spectranist ri

1501 (Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Lai, W.-C.; Song, C., Temperature-programmed retention indices for g. c. and g. c.-m. s. analysis of coal- and

petroleum-derived liquid fuels, Fuel, 74(10), 1995, 1436-1451., Program type: Ramp; Column cl… (show more)ass: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 6 K/min; Start T: 40 C; End T: 310 C; CAS no: 3321504; Active phase: DB-5; Carrier gas: He; Phase thickness: 0. 25 um; Data type: Linear RI; Authors: Song, C.; Lai, W.-C.; Madhusudan Reddy, K.; Wei, B., Chapter 7. Temperature-programmed retention indices for

GC and GC-MS of hydrocarbon fuels and simulated distillation GC of heavy oils, in Analytical advances for hydrocarbon research, Hsu, C. S., ed(s), Kluwer Academic/Plenum Publishers, New York, 2003, 147-193.)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:	272. 2±7. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 3 mmHg at 25°C
Enthalpy of Vaporization:	49. 0±0. 8 kJ/mol
Flash Point:	106. 7±11. 7 °C
Index of Refraction:	1. 466

Molar Refractivity:	62. 7±0. 3 cm^{3}
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	3
#Rule of 5 Violations:	1
ACD/LogP:	7. 00
ACD/LogD (pH 5. 5):	6. 07
ACD/BCF (pH 5. 5):	24105. 85
ACD/KOC (pH 5. 5):	47677. 00
ACD/LogD (pH 7. 4):	6. 07
ACD/BCF (pH 7. 4):	24105. 85
ACD/KOC (pH 7. 4):	47677. 00
Polar Surface Area:	0 $Å^{2}$
Polarizability:	24. 8±0. 5 10^{-24} cm^{3}
Surface Tension:	31. 6±3. 0 dyne/cm
Molar Volume:	226. 5±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) = 6. 85Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 258. 73 (Adapted Stein & Brown method)Melting Pt (deg C): 13. 27 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 0138 (Mean VP of Antoine & Grain methods)MP (exp database): 11. 5 deg CBP (exp database): 272. 5 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 01937log Kow used: 6. 85 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 039547 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 09E+000 atm-m3/moleGroup Method: 5. 11E-001 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 1. 822E-001 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 6. 85 (KowWin est)Log Kaw used: 1. 649 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 5. 201Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6550Biowin2 (Non-Linear Model) : 0. 5619Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7697 (weeks)Biowin4 (Primary Survey Model) : 3. 5673 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 4549Biowin6 (MITI Non-Linear Model): 0. 4700Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 2332Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 5647BioHC Half-Life (days) : 36. 7021Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 89 Pa (0. 0142 mm Hg)Log Koa (Koawin est): 5. 201Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 58E-006 Octanol/air (Koa) model: 3. 9E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 5. 72E-005 Mackay model : 0. 000127 Octanol/air (Koa) model: 3. 12E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 24. 1767 E-12 cm3/molecule-secHalf-Life = 0. 442 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 5. 309 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 9. 2E-005 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 2. 083E+004Log Koc: 4. 319 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 = 4. 571 (BCF = 3. 721e+004)log Kow used: 6. 85 (estimated)Volatilization from Water: Henry LC: 1. 09 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 1. 423 hoursHalf-Life from Model Lake : 132. 4 hours (5. 518 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 98. 38 percentTotal biodegradation: 0. 33 percentTotal sludge adsorption: 68. 36 percentTotal to Air: 29. 69 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 45 10. 6 1000 Water 4. 38 360 1000 Soil 29. 4 720 1000 Sediment 65. 8 3. 24e+003 0 Persistence Time: 1. 11e+003 hr

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