Nonane c9h20 structure

Contents

Molecular Formula	C_9H_{20}
Average mass	128. 255 Da
Density	0. 7±0. 1 g/cm ^{3}
Boiling Point	151. 7±3. 0 °C at 760 mmHg
Flash Point	31. 1±0. 0 °C
Molar Refractivity	43. 7±0. 3 cm ^{3}
Polarizability	17. 3±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension	23. 6±3. 0 dyne/cm
Molar Volume	177. 1±3. 0 cm ^{3}

- Experimental Physico-chemical Properties

Experimental Melting Point:

-53 °CAlfa Aesar

-53 °CIndofine[05-0900],[05-0900]

-53 °COxford University Chemical Safety Data (No longer updated)More details

-54 °CJean-Claude Bradley Open Melting Point Dataset13636

-53. 5 °CJean-Claude Bradley Open Melting Point Dataset20387

-53 °CJean-Claude Bradley Open Melting Point Dataset16021, 8111

-53 °CAlfa AesarA16177

0. 718 °CLabNetworkLN00164304

-53 °CIndofine[05-0900],[05-0900],[05-0900]

-51 °CFooDBFDB000757

Experimental Boiling Point:

150-152 °CAlfa Aesar

303 F (150. 5556 °C)NIOSHRA6115000

151 °COxford University Chemical Safety Data (No longer

updated)More details

150-152 °CAlfa AesarA16177

151 °CLabNetworkLN00164304

150. 8 °CFooDBFDB000757

- **Experimental Ionization Potent:**

  10. 21

  EvNIOSHRA6115000

- **Experimental Vapor Pressure:**

  3

  mmHgNIOSHRA611500

  0

- **Experimental Flash Point:**

  31 °CAlfa Aesar

  88 F (31. 1111 °C)NIOSHRA6115000

  31 °COxford University Chemical Safety Data (No longer

  updated)More details

  31 °CAlfa Aesar

  31 °F (-0. 5556 °C)Alfa AesarA16177

100 °CSynQuest52593, 8169-3-12

31 °COakwood098885

31 °CLabNetworkLN00164304

- **Experimental Freezing Point:**

  -60 F (-51. 1111

  °C)NIOSHRA6115000

- **Experimental Gravity:**

  20 g/mLMerck Millipore1679

  20 g/lMerck Millipore1679,

  806838

  0. 718 g/mLAlfa

  AesarA16177

  1. 15 g/mLSynQuest8169-3-

  12

- **Experimental Refraction Index:**

  1. 4054Alfa

  AesarA16177

- **Experimental Solubility:**

  InsolubleNIOSHRA61150

00

- Miscellaneous

Appearance:

Colorless liquid with a gasoline-like odor. NIOSHRA6115000

colourless liquidOxford University Chemical Safety Data (No longer updated)More details

Stability:

Stable. Highly flammable. Incompatible with strong oxidizing agents. Oxf

University Chemical Safety Data (No longer updated)More details

Safety:

10-20-65-66Alfa AesarA16177

23-36-62Alfa AesarA16177

3Alfa AesarA16177

DangerAlfa AesarA16177

DangerBiosynthW-108667

DANGER: FLAMMABLE, irritates skin, eyes, lungsAlfa AesarA16177

GHS02; GHS07; GHS08BiosynthW-108667

H226; H304; H315; H319; H332; H336BiosynthW-108667

H304-H226-H332-EUH066Alfa AesarA16177

IrritantSynQuest52593, 8169-3-12

P261; P301+P310; P305+P351+P338; P331BiosynthW-108667

P261-P280f-P301+P310-P315Alfa AesarA16177

Safety glasses, adequate ventilation. Oxford University Chemical Safety

longer updated)More details

- **First-Aid:**

  Eye: Irrigate immediately Skin: Soap wash immediately Breathing: Respi

  support Swallow: Medical attention immediatelyNIOSHRA6115000

- **Exposure Routes:**

  inhalation, ingestion, skin and/or eye

  contactNIOSHRA6115000

- **Symptoms:**

  Irritation eyes, skin, nose, throat; headache, drowsiness, dizziness, confu

  nausea, tremor, incoordination; chemical pneumonitis (aspiration

  liquid)NIOSHRA6115000

- **Target Organs:**

  Eyes, skin, respiratory system, central nervous

systemNIOSHRA6115000

- **Incompatibility:**

  Strong oxidizers (e. g., peroxides, nitrates, perchlorates)NIOSHRA6115000

- **Personal Protection:**

  Skin: No recommendation Eyes: Prevent eye contact Wash skin: Daily Re

  When wet (flammable) Change: No recommendation Provide: EyewashNIOSHRA6115000

- **Exposure Limits:**

  NIOSH REL : TWA 200 ppm (1050 mg/m 3) OSHA PEL ?: noneNIOSHRA6115000

- Gas Chromatography

  - **Retention Index (Kovats):**

    916 (estimated with error: 39)NIST Spectramainlib_228006, replib_2665, replib_249212

  - **Retention Index (Lee):**

    138. 27 (Program type: Ramp; Column cl… (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 10 K/min; Start T: 40 C; End T: 310 C; Start time: 1 min; CAS n 111842; Active phase: DB-5MS; Phase thickness: 0. 5 um; Data type: Lee Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.;

D. W., Application of Lee retention indices to the confirmation of tentativ identified compounds from GC/MS analysis of environmental samples, Te paper, Analytical Services Division, Environmental Science&Engineering, Box 1703, Gainesville, FL 32602, 2002, 11.)NIST Spectranist ri

144. 03 (Program type: Ramp; Column cl... (show more)ass: Semi-standa polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: C Heat rate: 4 K/min; Start T: 40 C; End T: 310 C; Start time: 1 min; CAS no 111842; Active phase: DB-5MS; Phase thickness: 0. 5 um; Data type: Lee Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.; D. W., Application of Lee retention indices to the confirmation of tentativ identified compounds from GC/MS analysis of environmental samples, Te paper, Analytical Services Division, Environmental Science&Engineering, Box 1703, Gainesville, FL 32602, 2002, 11.)NIST Spectranist ri

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

  900 (Column class: All column type... (show more)s; CAS no: 111842; Da Normal alkane RI value specified by scale definition; Authors: von Kovats Gas-chromatographische Charakterisierung organischer Verbindungen. T Retentionsindices aliphatischer Halogenide, Alkohole, Aldehyde und Keto Helv. Chim. Acta, 41(7), 1958, 1915-1932.)NIST Spectranist ri

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

Density:	0. 7±0. 1 g/cm ^{3}

Boiling Point:	151. 7±3. 0 °C at 760 mmHg
Vapour Pressure:	4. 6±0. 1 mmHg at 25°C
Enthalpy of Vaporization:	36. 9±0. 0 kJ/mol
Flash Point:	31. 1±0. 0 °C
Index of Refraction:	1. 409
Molar Refractivity:	43. 7±0. 3 cm^3
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	6
#Rule of 5 Violations:	1
ACD/LogP:	5. 54
ACD/LogD (pH 5. 5):	5. 30
ACD/BCF (pH 5. 5):	6231. 33
ACD/KOC (pH 5. 5):	18103. 10
ACD/LogD (pH 7. 4):	5. 30
ACD/BCF (pH 7. 4):	6231. 33

ACD/KOC (pH 7. 4):	18103. 10
Polar Surface Area:	0 Å ^{2}
Polarizability:	17. 3±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	23. 6±3. 0 dyne/cm
Molar Volume:	177. 1±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) = 4. 76Log Kow (Exper. database match) = 5. 65Exper. Ref: DAYLIGHT (2003)Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 142. 69 (Adapted Stein & Brown method)Melting Pt (deg C): -56. 16 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 4. 96 (Mean VP of Antoine & Grain methods)MP (exp database): -53. 5 deg CBP (exp database): 150. 8 deg CVP (exp database): 4. 45E+00 mm Hg at 25 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 4058log Kow used: 5. 65 (expkow database)no-melting pt equation usedWater Sol (Exper. database match) = 220 mg/L (25 deg C)Exper. Ref: RIDDICK, JA ET AL. (1986)Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 0. 28467 mg/LWat Sol (Exper. database match) = 220. 00Exper. Ref: RIDDICK, JA ET AL. (1986)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 4. 00E+000 atm-m3/moleGroup Method: 4. 77E+000 atm-m3/moleExper Database: 3. 40E+00 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 063E+000 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 65 (exp database)Log Kaw used: 2. 143 (exp database)Log Koa (KOAWIN v1. 10 estimate): 3. 507Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 9033Biowin2 (Non-Linear Model) : 0. 9924Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 5124 (days-weeks)Biowin4 (Primary Survey Model) : 4. 2008 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6773Biowin6 (MITI Non-Linear Model): 0. 8663Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 2234Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 0. 8713BioHC Half-Life (days) : 7. 4345Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 593 Pa (4. 45 mm Hg)Log Koa (Koawin est): 3. 507Kp (particle/gas partition coef. (m3/ug)): Mackay model : 5. 06E-009 Octanol/air (Koa) model: 7. 89E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 83E-007 Mackay model : 4. 04E-007 Octanol/air (Koa) model: 6. 31E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 9. 6974 E-12

cm3/molecule-secHalf-Life = 1. 103 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 13. 236 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 2. 94E-007 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 934. 6Log Koc: 2. 971 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. 651 (BCF = 447. 2)log Kow used: 5. 65 (expkow database)Volatilization from Water: Henry LC: 3. 4 atm-m3/mole (Henry experimental database)Half-Life from Model River: 1. 156 hoursHalf-Life from Model Lake : 107. 6 hours (4. 482 days)Removal In Wastewater Treatment (recommended maximum 95%): Total removal: 99. 92 percentTotal biodegradation: 0. 17 percentTotal sludge adsorption: 56. 95 percentTotal to Air: 42. 80 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 6. 78 25. 2 1000 Water 18. 3 208 1000 Soil 27. 7 416 1000 Sediment 47. 3 1. 87e+003 0 Persistence Time: 251 hr

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- 1-Click Scaffold Hop