

# [Nonane c9h20 structure](https://assignbuster.com/nonane-c9h20-structure/)

Contents

* Retention Index (Normal Alkane):

|  |  |
| --- | --- |
| Molecular Formula  | C 9 H 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 data
* Predicted – ACD/Labs
* Predicted – EPISuite
* Predicted – ChemAxon
* Predicted – Mcule
* 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| -53 °COxford University Chemical Safety Data (No longer updated)More details  |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| 151 °COxford University Chemical Safety Data (No longer updated)More details  |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 mmHgNIOSHRA6115000  |

## 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| 31 °COxford University Chemical Safety Data (No longer updated)More details  |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:

|  |
| --- |
| InsolubleNIOSHRA6115000  |

* Miscellaneous

## Appearance:

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| --- |
| 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. Oxford 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 Data (No longer updated)More details  |

## First-Aid:

|  |
| --- |
| Eye: Irrigate immediately Skin: Soap wash immediately Breathing: Respiratory support Swallow: Medical attention immediatelyNIOSHRA6115000  |

## Exposure Routes:

|  |
| --- |
| inhalation, ingestion, skin and/or eye contactNIOSHRA6115000  |

## Symptoms:

|  |
| --- |
| Irritation eyes, skin, nose, throat; headache, drowsiness, dizziness, confusion, nausea, tremor, incoordination; chemical pneumonitis (aspiration liquid)NIOSHRA6115000  |

## Target Organs:

|  |
| --- |
| Eyes, skin, respiratory system, central nervous systemNIOSHRA6115000  |

## Incompatibility:

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

## Personal Protection:

|  |
| --- |
| Skin: No recommendation Eyes: Prevent eye contact Wash skin: Daily Remove: 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-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Heat rate: 10 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 RI; Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.; Roberts, D. W., Application of Lee retention indices to the confirmation of tentatively identified compounds from GC/MS analysis of environmental samples, Technical paper, Analytical Services Division, Environmental Science&Engineering, Inc, PO Box 1703, Gainesville, FL 32602, 2002, 11.)NIST Spectranist ri  |
| 144. 03 (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: 1 min; CAS no: 111842; Active phase: DB-5MS; Phase thickness: 0. 5 um; Data type: Lee RI; Authors: Chen, P. H.; Keeran, W. S.; Van Ausdale, W. A.; Schindler, D. R.; Roberts, D. W., Application of Lee retention indices to the confirmation of tentatively identified compounds from GC/MS analysis of environmental samples, Technical paper, Analytical Services Division, Environmental Science&Engineering, Inc, PO 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; Data type: Normal alkane RI value specified by scale definition; Authors: von Kovats, E., 206. Gas-chromatographische Charakterisierung organischer Verbindungen. Teil 1: Retentionsindices aliphatischer Halogenide, Alkohole, Aldehyde und Ketone, 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