

1,2,3,4,5,6,7,8-  
octahydrophenanthre  
ne c14h18 structure



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\n[[toc title="Table of Contents"](#)]\n

\n \t

1. [Experimental Melting Point:](#) \n \t
2. [Retention Index \(Kovats\):](#) \n \t
3. [Retention Index \(Lee\):](#) \n \t
4. [Retention Index \(Normal Alkane\):](#) \n \t
5. [Retention Index \(Linear\):](#) \n

\n[/toc]\n \n

## Contents

- Retention Index (Linear):

Molecular

$C_{14}H_{18}$

Formula

Average mass 186. 293 Da

Density  $1. 0\pm 0. 1 \text{ g/cm}^3$

Boiling Point  $295. 0\pm 0. 0 \text{ }^\circ\text{C}$  at  
760 mmHg

Flash Point  $132. 2\pm 14. 5 \text{ }^\circ\text{C}$

Molar  
Refractivity  $59. 8\pm 0. 3 \text{ cm}^3$

Polarizability  $23. 7\pm 0. 5 \cdot 10^{-24}$

cm<sup>3</sup>

Surface 39.8 ± 3.0

Tension dyne/cm

Molar Volume 183.1 ± 3.0 cm<sup>3</sup>

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

- **Experimental Melting Point:**

16.7 °C Jean-Claude

Bradley Open Melting

Point Dataset24097

- Gas Chromatography

- **Retention Index (Kovats):**

1652 (estimated with

error: 55) NIST

Spectramainlib\_2297

66, replib\_27673,

replib\_157405

1716 (Program type:

Isothermal; Col...

(show more)umn

class: Standard non-

polar; Column

diameter: 0.5 mm;

Column length: 100

m; Column type:

Capillary; Start T:

175 C; CAS no:

5325973; Active

phase: SE-30; Data

type: Kovats RI;

Authors: Bredael, P.,

Retention indices of

hydrocarbons on SE-

30, J. Hi. Res.

Chromatogr. &

Chromatogr. Comm.,

5, 1982, 325-

328.)NIST

Spectranist ri

1694 (Program type:

Isothermal; Col...

(show more)umn

class: Standard non-polar; Column type: Packed; Start T: 150 C; CAS no: 5325973; 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 identification of hydrocarbons by gas chromatography from temperature coefficients of retention indices, Zh. Anal. Khim., 30, 1975, 788-792.)NIST Spectranist ri 1731 (Program type: Isothermal; Col... (show more)umn

class: Standard non-polar; Column type: Packed; Start T: 200 C; CAS no: 5325973; 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 identification of hydrocarbons by gas chromatography from temperature coefficients of retention indices, Zh. Anal. Khim., 30, 1975, 788-792.)NIST Spectranist ri 1765 (Program type: Isothermal; Col... (show more)umn

class: Semi-standard

non-polar; Column

type: Packed; Start

T: 150 C; CAS no:

5325973; 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 identification

of hydrocarbons by

gas chromatography

from temperature

coefficients of

retention indices, Zh.

Anal. Khim., 30,

1975, 788-792.)NIST

Spectranist ri

- **Retention Index (Lee):**

292. 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:  
15 K/min; Start T: 50  
C; End T: 300 C; CAS  
no: 5325973; Active  
phase: DB-5; Phase  
thickness: 0. 25 um;  
Data type: Lee RI;  
Authors: Durlak, S.  
K.; Biswas, P.; Shi, J.;  
Bernhard, M. J.,  
Characterization of  
polycyclic aromatic  
hydrocarbon  
particulate and  
gaseous emissions  
from polystyrene



combustion, Environ.  
Sci. Technol., 32,  
1998, 2301-  
2307.)NIST  
Spectranist ri  
  
291. 63 (Program  
type: Ramp; Column  
cl... (show more)ass:  
Semi-standard non-  
polar; Column  
diameter: 0. 22 mm;  
Column length: 20  
m; Column type:  
Capillary; Heat rate:  
4 K/min; Start T: 50  
C; End T: 300 C; CAS  
no: 5325973; Active  
phase: SE-54; Carrier  
gas: He; Phase  
thickness: 0. 20 um;  
Data type: Lee RI;  
Authors: Guillen, M.  
D.; Blanco, J.;  
Bermejo, J.; Blanco,  
C. G., Temperature

programmed  
retention indices of  
some PAHs on  
Capillary columns  
coated with OV-1701  
and SE-54, J. Hi. Res.  
Chromatogr., 12,  
1989, 552-554.)NIST  
Spectranist ri

291. 4 (Program  
type: Ramp; Column  
cl... (show more)ass:  
Semi-standard non-  
polar; Column type:  
Capillary; CAS no:  
5325973; Active  
phase: SE-52; Data  
type: Lee RI;  
Authors: Shlyakhov,  
A. F., Gas  
chromatography in  
organic  
geochemistry, Nedra,  
Moscow, 1984,  
221.)NIST

Spectranist ri

292. 03 (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: 5325973; 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., Program  
type: Ramp; Column  
cl... (show more)ass:  
Semi-standard non-  
polar; Column type:  
Capillary; CAS no:  
5325973; Active  
phase: SE-52; Data  
type: Lee RI;  
Authors: Shlyakhov,  
A. F., Gas  
chromatography in  
organic  
geochemistry, Nedra,  
Moscow, 1984,  
221.)NIST  
Spectranist ri

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

1696 (Program type:

Ramp; Column cl...

(show more)ass:

Standard non-polar;

Column diameter: 0.

2 mm; Column

length: 50 m;

Column type:

Capillary; Heat rate:

3 K/min; Start T: 60

C; End T: 300 C; End

time: 35 min; CAS

no: 5325973; Active

phase: Ultra-1;

Carrier gas: H<sub>2</sub>;

Phase thickness: 0.

33 um; Data type:

Normal alkane RI;

Authors: Elizalde-

Gonzalez, M. P.;

Hutfließ, M.;

Hedden, K.,

Retention index

system, adsorption

characteristics, and

structure correlations

of polycyclic

aromatic  
hydrocarbons in  
fuels, J. Hi. Res.  
Chromatogr., 19,  
1996, 345-352.)NIST  
Spectranist ri

1720 (Program type:

Isothermal; Col...

(show more)umn

class: Standard non-

polar; Column type:

Packed; Start T: 183

C; CAS no: 5325973;

Active phase:

Polydimethyl

siloxane; Data type:

Normal alkane RI;

Authors: Ferrand, R.,

Gas phase

chromatography

using retention

indices for the

analysis of tars and

their hydrogenation

products, Journees

internationales  
d'étude des  
methodes de  
separation  
immediate at de  
chromatographie;  
Org. sur l'initiative  
du IX., , 1962, 132-  
140.)NIST  
Spectranist ri

- **Retention Index (Linear):**

1705. 5 (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: 5325973; Active  
phase: DB-5; Carrier

gas: He; Phase  
thickness: 0.25 µm;  
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: 5325973; Active



phase: DB-5; Carrier

gas: He; Phase

thickness: 0.25 µm;

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

1721. 1 (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: 5325973; 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: 5325973; 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

1730. 6 (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: 5325973; Active  
phase: DB-5; Carrier  
gas: He; Phase

thickness: 0.25 µm;  
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: 5325973; 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  
1693 (Program type:  
Ramp; Column cl...

(show more)ass:

Semi-standard non-

polar; Column

diameter: 0. 50 mm;

Column length: 33. 3

m; Column type:

Capillary; Heat rate:

6 K/min; Start T: 50

C; End T: 320 C;

Start time: 5 min;

CAS no: 5325973;

Active phase: SE-52;

Carrier gas: He; Data

type: Linear RI;

Authors: Beernaert,

H., Gas

Chromatographic

Analysis of Polycyclic

Aromatic

Hydrocarbons, J.

Chromatogr., 173,

1979, 109-118.)NIST

Spectranist ri

Predicted data is generated using the ACD/Labs Percepta Platform -

PhysChem Module

<https://assignbuster.com/12345678-octahydrophenanthrene-c14h18-structure/>

Density:	1. 0±0. 1 g/cm <sup>3</sup>
Boiling Point:	295. 0±0. 0 °C at 760 mmHg
Vapour Pressure:	0. 0±0. 3 mmHg at 25°C
Enthalpy of Vaporization:	51. 3±0. 8 kJ/mol
Flash Point:	132. 2±14. 5 °C
Index of Refraction:	1. 567
Molar Refractivity:	59. 8±0. 3 cm <sup>3</sup>
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	0
#Rule of 5 Violations:	1
ACD/LogP:	5. 59
ACD/LogD (pH 5. 5):	5. 09
ACD/BCF (pH 5. 5):	4342. 43
ACD/KOC (pH 5. 5):	13979. 21
ACD/LogD (pH 7. 4):	5. 09



ACD/BCF (pH 7. 4):	4342. 43
ACD/KOC (pH 7. 4):	13979. 21
Polar Surface Area:	0 Å <sup>2</sup>
Polarizability:	23. 7±0. 5 10 <sup>-24</sup> cm <sup>3</sup>
Surface Tension:	39. 8±3. 0 dyne/cm
Molar Volume:	183. 1±3. 0 cm <sup>3</sup>

Predicted data is generated using the US Environmental Protection Agency's  
EPISuite™

Log Octanol-Water Partition Coef (SRC): Log Kow (KOWWIN v1. 67 estimate) = 5. 09Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 275. 18 (Adapted Stein & Brown method)Melting Pt (deg C): 46. 90 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 00785 (Modified Grain method)Subcooled liquid VP: 0. 0125 mm Hg (25 deg C, Mod-Grain method)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 0. 6687log Kow used: 5. 09 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 4. 8432 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 2. 08E-001 atm-m3/moleGroup Method: 6. 14E-004 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 2. 878E-003 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 5. 09 (KowWin est)Log Kaw used: 0. 930 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 160Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 6589Biowin2 (Non-Linear Model) : 0. 5898Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 7875 (weeks )Biowin4 (Primary Survey Model) : 3. 5790 (days-weeks )MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 3343Biowin6 (MITI Non-Linear Model): 0. 2942Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3446Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 1. 7617BioHC Half-Life (days) : 57. 7683Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 1. 67 Pa (0. 0125 mm Hg)Log Koa (Koawin est ): 4. 160Kp (particle/gas partition coef. (m3/ug)): Mackay model : 1. 8E-006 Octanol/air (Koa) model: 3. 55E-009 Fraction sorbed

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to airborne particulates (phi): Junge-Pankow model : 6. 5E-005 Mackay model : 0. 000144 Octanol/air (Koa) model: 2. 84E-007 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 255. 0644 E-12 cm<sup>3</sup>/molecule-secHalf-Life = 0. 042 Days (12-hr day; 1. 5E6 OH/cm<sup>3</sup>)Half-Life = 0. 503 HrsOzone Reaction: OVERALL Ozone Rate Constant = 410. 844971 E-17 cm<sup>3</sup>/molecule-secHalf-Life = 0. 003 Days (at 7E11 mol/cm<sup>3</sup>)Half-Life = 4. 017 MinFraction sorbed to airborne particulates (phi): 0. 000104 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 5586Log Koc: 3. 747 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 = 3. 220 (BCF = 1660)log Kow used: 5. 09 (estimated)Volatilization from Water: Henry LC: 0. 000614 atm-m<sup>3</sup>/mole (estimated by Group SAR Method)Half-Life from Model River: 2. 694 hoursHalf-Life from Model Lake : 143. 8 hours (5. 993 days)Removal In Wastewater Treatment: Total removal: 81. 73 percentTotal biodegradation: 0. 66 percentTotal sludge adsorption: 77. 50 percentTotal to Air: 3. 57 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 00796 0. 0628 1000 Water 13. 4 360 1000 Soil 68 720 1000 Sediment 18. 5 3. 24e+003 0 Persistence Time: 508 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop