

Squalane $C_{30}H_{62}$ structure



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Contents

- Retention Index (Linear):

Molecular

 $C_{30}H_{62}$

Formula

Average mass 422. 813 Da

Density $0.8 \pm 0.1 \text{ g/cm}^3$ Boiling Point $470.3 \pm 0.0 \text{ }^\circ\text{C}$ at
760 mmHgFlash Point $217.8 \pm 0.0 \text{ }^\circ\text{C}$ Molar
Refractivity $140.8 \pm 0.3 \text{ cm}^3$ Polarizability $55.8 \pm 0.5 \cdot 10^{-24}$
 cm^3 Surface
Tension $28.0 \pm 3.0 \text{ dyne/cm}$ Molar Volume $526.0 \pm 3.0 \text{ cm}^3$

- Experimental data
- Predicted - ACD/Labs
- Predicted - EPISuite

- Predicted - ChemAxon
- Experimental Physico-chemical Properties

- **Experimental Melting Point:**

-38 °C Alfa Aesar

-38 °C Oxford University

Chemical Safety Data

(No longer

updated) More details

-38 °C Jean-Claude

Bradley Open Melting

Point Dataset 15187,

20416, 8422

-38 °C Alfa

Aesar A17931

-38 °C

(Literature) LabNetwork

LN00195308

- **Experimental Boiling Point:**

210-215 deg C / 1 mm

(500. 0104-507. 7479

°C / 760 mmHg) Alfa

Aesar

210-215 °C Oxford

University Chemical

Safety Data (No longer

updated) More details

210-215 °C / 1 mm

(500. 0104-507. 7479

°C / 760 mmHg) Alfa

Aesar A17931

- **Experimental Flash Point:**

218 °C Alfa Aesar

217 °C Oxford

University Chemical

Safety Data (No longer

updated) More details

218 °C Alfa Aesar

218 °F (103. 3333

°C) Alfa Aesar A17931

424

°C LabNetwork LN00195

308

- **Experimental Gravity:**

20 g/mL Merck Millipore 2544

20 g/L Merck Millipore 2544,

814605

0.81 g/mL Alfa Aesar A17931

- **Experimental Refraction Index:**

1.451 Alfa

Aesar A17931

- Miscellaneous

- **Appearance:**

viscous colourless

liquid Oxford University

Chemical Safety Data

(No longer

updated) More details

- **Stability:**

Stable. Combustible.

Incompatible

with strong oxidizing

agents. Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Safety:**

26-37Alfa AesarA17931

36/37/38Alfa

AesarA17931

GHS07BiosynthW-

109407

H315; H319;

H335BiosynthW-

109407

H315-H319-H335Alfa

AesarA17931

P261;

P305+P351+P338Biosy

nthW-109407

P261-P280-

P305+P351+P338-

P304+P340-P405-

P501aAlfa

AesarA17931

Safety glasses. Oxford

University Chemical

Safety Data (No longer

updated)More details

WarningAlfa

AesarA17931

WarningBiosynthW-

109407

WARNING: Irritates

lungs, eyes, skinAlfa

AesarA17931

- Gas Chromatography

- **Retention Index (Kovats):**

2619 (estimated with

error: 39)NIST

Spectramainlib_62218,

replib_17348,

replib_227596

2665 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;
Column diameter: 0. 21
mm; Column length:
17. 5 m; Column type:
Capillary; Start T: 240
C; CAS no: 111013;
Active phase: SE-30;
Carrier gas: He; Data
type: Kovats RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.
Anal. Khim., 43, 1988,
1082-1088., Program
type: Isothermal; Col...
(show more)umn class:
Standard non-polar;
Column diameter: 0. 21
mm; Column length:

17.5 m; Column type:
Capillary; Start T: 260
C; CAS no: 111013;
Active phase: SE-30;
Carrier gas: He; Data
type: Kovats RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.
Anal. Khim., 43, 1988,
1082-1088.)NIST
Spectranist ri

2666 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column diameter: 0.21
mm; Column length:

17.5 m; Column type:
Capillary; Start T: 240
C; CAS no: 111013;
Active phase: SE-30;
Carrier gas: He; Data
type: Kovats RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.
Anal. Khim., 43, 1988,
1082-1088., Program
type: Isothermal; Col...
(show more)umn class:
Standard non-polar;
Column diameter: 0.21
mm; Column length:
17.5 m; Column type:
Capillary; Start T: 260
C; CAS no: 111013;

Active phase: SE-30;

Carrier gas: He; Data

type: Kovats RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

capillary columns with

chemically immobilized

stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2667 (Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Start T: 240

C; CAS no: 111013;

Active phase: SE-30;

Carrier gas: He; Data

type: Kovats RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

capillary columns with

chemically immobilized

stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2657 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Start T: 240

C; CAS no: 111013;

Active phase: SE-52;

Carrier gas: He; Data

type: Kovats RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

capillary columns with

chemically immobilized

stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2658. 1 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Start T: 260

C; CAS no: 111013;

Active phase: SE-52;

Carrier gas: He; Data

type: Kovats RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

capillary columns with

chemically immobilized

stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2658. 5 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Start T: 260

C; CAS no: 111013;

Active phase: SE-52;
Carrier gas: He; Data
type: Kovats RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.
Anal. Khim., 43, 1988,
1082-1088.)NIST
Spectranist ri

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

2663 (Program type:
Complex; Column...
(show more)class:
Standard non-polar;
Column diameter: 0. 32
mm; Column length: 25
m; Column type:
Capillary; Description:

50C=> 20C/min =>
130C => 4C/min =>
300C (20min); CAS no:
111013; Active phase:
CP Sil 5 CB; Carrier
gas: He; Phase
thickness: 0.2 um;
Data type: Normal
alkane RI; Authors:
Kenig, F.; Sinninghe
Damste, J. S.; Kock-van
Dalen, A. C.; Rijpstra,
W. I. C.; Huc, A. Y.; de
Leeuw, J. W.,
Occurrence and origin
of mono-, di-, and
trimethylalkanes in
modern and holocene
cyanobacterial mats
from Abu Dhabi, United
Arab Emirates,
Geochim. Cosmochim.
Acta, 59(14), 1995,
2999-3015.)NIST
Spectranist ri

2668 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 21
mm; Column length: 25
m; Column type:
Capillary; Heat rate: 6
K/min; Start T: 40 C;
End T: 280 C; CAS no:
111013; Active phase:
SE-30; Carrier gas: He;
Data type: Normal
alkane RI; Authors:
Pozhidaev, V. M.;
Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhideava,
Capillary
chromatography of
polycyclic aromatic
hydrocarbons on a
home-produced
capillary column with
immobilized stationary
liquid phase SE-30, Zh.

Anal. Khim., 62(12),
1987, 2222-2226.)NIST

Spectranist ri

2657 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column diameter: 0. 21
mm; Column length:
17. 5 m; Column type:
Capillary; Start T: 240
C; CAS no: 111013;
Active phase: SE-52;
Carrier gas: He; Data
type: Normal alkane RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2658. 8 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Start T: 260

C; CAS no: 111013;

Active phase: SE-52;

Carrier gas: He; Data

type: Normal alkane RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

capillary columns with

chemically immobilized

stationary phases, Zh.

Anal. Khim., 43, 1988,

1082-1088.)NIST

Spectranist ri

2630 (Program type:

Ramp; Column cl...

(show more)ass: Semi-

standard non-polar;

Column type: Capillary;

CAS no: 111013; Active

phase: Apiezon; Data

type: Normal alkane RI;

Authors: Petrov, A. A.,

Hydrocarbons of

petroleum, Nauka

(publishing house),

Moscow, 1984, 263.,

Program type: Ramp;

Column cl... (show

more)ass: Semi-

standard non-polar;

Column type: Capillary;

Heat rate: 2 K/min;

Start T: 130 C; End T:

300 C; CAS no:

111013; Active phase:

Apiezon L; Data type:
Normal alkane RI;
Authors: Shlyakhov, A.
F., Gas
chromatography in
organic geochemistry,
Nedra, Moscow, 1984,
221.)NIST Spectranist ri

2632 (Program type:
Ramp; Column cl...
(show more)ass: Semi-
standard non-polar;
Column type: Capillary;
CAS no: 111013; Active
phase: Apiezon; Data
type: Normal alkane RI;
Authors: Petrov, A. A.,
Hydrocarbons of
petroleum, Nauka
(publishing house),
Moscow, 1984,
263.)NIST Spectranist ri

- **Retention Index (Linear):**

2664. 4 (Program type:

Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 21
mm; Column length:
17. 5 m; Column type:
Capillary; Heat rate: 2
K/min; Start T: 100 C;
End T: 280 C; CAS no:
111013; Active phase:
SE-30; Carrier gas: He;
Data type: Linear RI;
Authors: Pozhidaev, V.
M.; Berezkin, V. G.;
Korolev, A. A.; Popova,
T. P.; Pozhidaeva, K. A.,
Retention indices of
polycyclic aromatic
hydrocarbons on quartz
capillary columns with
chemically immobilized
stationary phases, Zh.
Anal. Khim., 43, 1988,
1082-1088.)NIST
Spectranist ri

2663 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column diameter: 0. 20
mm; Column length:
12. 5 m; Column type:
Capillary; Heat rate: 5
K/min; Start T: 120 C;
End T: 325 C; End time:
5 min; CAS no: 111013;
Active phase: Ultra-1;
Carrier gas: He; Phase
thickness: 0. 11 um;
Data type: Linear RI;
Authors: Tokuda, H.;
Saitoh, E.; Kimura, Y.;
Takano, S., Automated
analysis of various
compounds with a wide
range of boiling points
by capillary gas
chromatography based
on retention indices, J.
Chromatogr., 454,
1988, 109-120.)NIST

Spectranist ri

2660 (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: 50 C;

End T: 260 C; Start

time: 3 min; CAS no:

111013; Active phase:

HP-5; Carrier gas: He;

Phase thickness: 0. 25

um; Data type: Linear

RI; Authors: Zhao, Y. P.;

Wang X. Y.; Wang, Z.

C.; Lu Y.; Fu, C. X.;

Chen, S. Y., Essential

oil of Actinidia

macrosperma, a catnip

response kiwi endemic

to China, Journal of

Zhejiang University

SCIENCE B, 7(9), 2006,

708-712.)NIST

Spectranist ri

2656. 1 (Program type:

Ramp; Column cl...

(show more)ass: Semi-

standard non-polar;

Column diameter: 0. 21

mm; Column length:

17. 5 m; Column type:

Capillary; Heat rate: 2

K/min; Start T: 100 C;

End T: 280 C; CAS no:

111013; Active phase:

SE-52; Carrier gas: He;

Data type: Linear RI;

Authors: Pozhidaev, V.

M.; Berezkin, V. G.;

Korolev, A. A.; Popova,

T. P.; Pozhidaeva, K. A.,

Retention indices of

polycyclic aromatic

hydrocarbons on quartz

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Anal. Khim., 43, 1988,

1082-1088.)NIST

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

Density:	0.8±0.1 g/cm ³
Boiling Point:	470.3±0.0 °C at 760 mmHg
Vapour Pressure:	0.0±0.5 mmHg at 25°C
Enthalpy of Vaporization:	70.5±0.8 kJ/mol
Flash Point:	217.8±0.0 °C
Index of Refraction:	1.448
Molar Refractivity:	140.8±0.3 cm ³
#H bond acceptors:	0
#H bond donors:	0
#Freely Rotating Bonds:	21
#Rule of 5 Violations:	1
ACD/LogP:	15.59

ACD/LogD (pH 5. 5):	13. 46
ACD/BCF (pH 5. 5):	1000000. 00
ACD/KOC (pH 5. 5):	10000000. 00
ACD/LogD (pH 7. 4):	13. 46
ACD/BCF (pH 7. 4):	1000000. 00
ACD/KOC (pH 7. 4):	10000000. 00
Polar Surface Area:	0 Å ²
Polarizability:	55. 8±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	28. 0±3. 0 dyne/cm
Molar Volume:	526. 0±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) = 14. 63Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 408. 49 (Adapted Stein & Brown method)Melting Pt (deg C): 74. 73 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 000275 (Modified Grain method)MP (exp database): -38 deg CBP (exp database): 350 deg CWater Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 2. 042e-010log Kow used: 14. 63 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 4. 2283e-007 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 53E+003 atm-m3/moleGroup Method: 2. 03E+004 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 7. 493E+005 atm-m3/moleLog Octanol-Air Partition

<https://assignbuster.com/squalane-c30h62-structure/>

Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 14. 63 (KowWin est)Log Kaw used: 4. 796 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 9. 834Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 5462Biowin2 (Non-Linear Model) : 0. 0476Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 2. 2648 (weeks-months)Biowin4 (Primary Survey Model) : 3. 2377 (weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : -0. 0559Biowin6 (MITI Non-Linear Model): 0. 0372Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): -0. 3798Ready Biodegradability Prediction: NOHydrocarbon Biodegradation (BioHCwin v1. 01): LOG BioHC Half-Life (days) : 2. 5230BioHC Half-Life (days) : 333. 4541Sorption to aerosols (25 Dec C) [AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 0. 0367 Pa (0. 000275 mm Hg)Log Koa (Koawin est): 9. 834Kp (particle/gas partition coef. (m3/ug)): Mackay model : 8. 18E-005 Octanol/air (Koa) model: 0. 00167 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 0. 00295 Mackay model : 0. 0065 Octanol/air (Koa) model: 0. 118 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 40. 4595 E-12 cm3/molecule-secHalf-Life = 0. 264 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 172 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 0. 00472 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 1. 494E+008Log Koc: 8. 174 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 = 0. 500 (BCF = 3. 162)log Kow used: 14. 63 (estimated)Volatilization from Water: Henry LC: 1. 53E+003 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 2. 098 hoursHalf-Life from Model Lake : 195. 3 hours (8. 138 days)Removal In Wastewater Treatment: Total removal: 94. 04 percentTotal biodegradation: 0. 78 percentTotal sludge adsorption: 93. 25 percentTotal to Air: 0. 00 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 0902 6. 35 1000 Water 1. 9 900 1000 Soil 27. 9 1. 8e+003 1000 Sediment 70. 1 8. 1e+003 0 Persistence Time: 3. 1e+003 hr