1-hexen-6-ol c6h12o structure

Contents

- Retention Index (Linear):

Molecular Formula	$C_6H_{12}O$
Average mass	100. 159 Da
Density	0. 8±0. 1 g/cm ^{3}
Boiling Point	149. 9±19. 0 °C at 760 mmHg
Flash Point	47. 2±0. 0 °C
Molar Refractivity	31. 1±0. 3 cm ^{3}
Polarizability	12. 3±0. 5 10^{-24} cm ^{3}
Surface Tension	28. 1±3. 0 dyne/cm
Molar Volume	120. 2±3. 0 cm ^{3}

- Experimental data
- Predicted – ACD/Labs

- Predicted – EPISuite
- Predicted – ChemAxon
- Experimental Physico-chemical Properties

Experimental Melting Point:

<-20 °CSynQuest

<-20 °CAlfa Aesar

<-20 °CAlfa AesarA15766

<-20 °CSynQuest55305,

2301-1-06

-20 °CBiosynthQ-200544

Experimental Boiling Point:

152-155 °CAlfa

Aesar

154-155 °CFood and

Agriculture

Organization of the

United Nations5-

Hexenol

152-155 °CAlfa

AesarA15766

157

°CSynQuest55305,

2301-1-06

78-80 °C / 25 mm

(191. 7254-194.

3129 °C / 760

mmHg)Oakwood[07

8461]

- **Experimental Flash Point:**

  59 °CAlfa Aesar

  59 °CAlfa Aesar

  47 °CBiosynthQ-200544

  59 °F (15 °C)Alfa

  AesarA15766

  47 °CSynQuest55305,

  2301-1-06

  47 °COakwood[078461]

- **Experimental Gravity:**

  20 g/mLMerck Millipore2439

20 g/lMerck Millipore2439,

814341

0. 834 g/mLBiosynthQ-

200544

15 g/mLSynQuest2301-1-06

0. 842 g/mLAlfa

AesarA15766

0. 85 g/mLSynQuest2301-1-

06

0. 834

g/mLOakwood[078461]

47 g/mLBiosynthQ-200544

- **Experimental Refraction Index:**

1. 435Alfa

AesarA15766

1. 434-1. 437Food

and Agriculture

Organization of the

United Nations5-

Hexenol

1.

436SynQuest55305,

2301-1-06

- Miscellaneous

- **Appearance:**

  Colourless liquid;

  Green aromaFood

  and Agriculture

  Organization of the

  United Nations5-

  Hexenol

  Not

  AvailableNovochemy

  [NC-18929]

- **Safety:**

  20/21/22Novochemy

  [NC-18929]

  20/21/36/37/39Novo

  chemy[NC-18929]

  26-36/37/39-45Alfa

AesarA15766

3Alfa AesarA15766

34Alfa AesarA15766

DangerAlfa

AesarA15766

DANGER:

FLAMMABLE,

CORROSIVE, burns

skin and eyesAlfa

AesarA15766

DANGER:

FLAMMABLE,

irritates skin and

eyesAlfa

AesarA15766

Flammable/

CorrosiveSynQuest2

301-1-06, 55305

GHS02BiosynthQ-

200544

GHS07;

GHS09Novochemy[N

C-18929]

H226BiosynthQ-

200544

H314-H226Alfa

AesarA15766

H332;

H403Novochemy[NC

-18929]

IRRITANTMatrix

Scientific074794

P210;

P280BiosynthQ-

200544

P210-P260-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

AesarA15766

P305+P351+P338;

P376;

P270Novochemy[NC

-18929]

R10,

R36/37/38SynQuest

2301-1-06, 55305

R52/53Novochemy[

NC-18929]

S26,

S36/37/39SynQuest

2301-1-06, 55305

WarningBiosynthQ-

200544

WarningNovochemy[

NC-18929]

- Gas Chromatography

  - **Retention Index (Kovats):**

    850 (estimated with

    error: 41)NIST

    Spectramainlib_352

    732, replib_288423,

    replib_1067

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

  1394 (Program type:

  Ramp; Column cl…

  (show more)ass:

  Standard polar;

  Column diameter: 0.

  25 mm; Column

  length: 50 m;

  Column type:

  Capillary; Heat rate:

  2 K/min; Start T: 60

  C; End T: 180 C;

  Start time: 4 min;

  CAS no: 821410;

  Active phase:

  Carbowax 20M;

  Carrier gas: He;

  Data type: Normal

  alkane RI; Authors:

  Kawakami, M.;

  Kobayashi, A.; Kator,

  K., Volatile

  constituents of

  Rooibos tea

  (Aspalathus linearis)

  as affected by

extraction process, J. Agric. Food Chem., 41(4), 1993, 633-636.)NIST Spectranist ri

- **Retention Index (Linear):**

878. 6 (Program type: Complex; Column… (show more)class: Semi-standard non-polar; Column diameter: 0. 25 mm; Column length: 30 m; Column type: Capillary; Description: Multi-step temperature program; T(initial)= 60C; T(final)= 270C; CAS no: 821410; Active phase: VF-5MS; Carrier gas: He; Phase thickness: 0. 25 um; Data type:

Linear RI; Authors:

Tret’yakov, K. V.,

Retention Data. NIST

Mass Spectrometry

Data Center.,

2008.)NIST

Spectranist ri

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

Density:	0. 8±0. 1 g/cm ^{3}
Boiling Point:	149. 9±19. 0 °C at 760 mmHg
Vapour Pressure:	1. 5±0. 6 mmHg at 25°C
Enthalpy of Vaporization:	45. 1±6. 0 kJ/mol
Flash Point:	47. 2±0. 0 °C
Index of Refraction:	1. 431
Molar Refractivity:	31. 1±0. 3 cm ^{3}
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	4

#Rule of 5 Violations:	0
ACD/LogP:	1. 50
ACD/LogD (pH 5. 5):	1. 36
ACD/BCF (pH 5. 5):	6. 35
ACD/KOC (pH 5. 5):	130. 74
ACD/LogD (pH 7. 4):	1. 36
ACD/BCF (pH 7. 4):	6. 35
ACD/KOC (pH 7. 4):	130. 74
Polar Surface Area:	20 Å ^{2}
Polarizability:	12. 3±0. 5 10 $^{-24}$ cm ^{3}
Surface Tension:	28. 1±3. 0 dyne/cm
Molar Volume:	120. 2±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) = 1. 69Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42): Boiling Pt (deg C): 157. 47 (Adapted Stein & Brown method)Melting Pt (deg C): -39. 22 (Mean or Weighted MP)VP(mm Hg, 25 deg C): 0. 887 (Mean VP of Antoine & Grain methods)Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water

Solubility at 25 deg C (mg/L): 1. 371e+004log Kow used: 1. 69 (estimated)no-melting pt equation usedWater Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 7237. 7 mg/LECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Neutral OrganicsHenrys Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 1. 31E-005 atm-m3/moleGroup Method: 6. 14E-006 atm-m3/moleHenrys LC [VP/WSol estimate using EPI values]: 8. 526E-006 atm-m3/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 69 (KowWin est)Log Kaw used: -3. 271 (HenryWin est)Log Koa (KOAWIN v1. 10 estimate): 4. 961Log Koa (experimental database): NoneProbability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8586Biowin2 (Non-Linear Model) : 0. 9373Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 1378 (weeks)Biowin4 (Primary Survey Model) : 3. 8327 (days)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 7915Biowin6 (MITI Non-Linear Model): 0. 9200Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 8522Ready Biodegradability Prediction: YESHydrocarbon Biodegradation (BioHCwin v1. 01): Structure incompatible with current estimation method! Sorption to aerosols (25 Dec C)[AEROWIN v1. 00]: Vapor pressure (liquid/subcooled): 106 Pa (0. 792 mm Hg)Log Koa (Koawin est): 4. 961Kp (particle/gas partition coef. (m3/ug)): Mackay model : 2. 84E-008 Octanol/air (Koa) model: 2. 24E-008 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 1. 03E-006 Mackay model : 2. 27E-006 Octanol/air (Koa) model: 1. 8E-006 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 34. 4358 E-12 cm3/molecule-secHalf-Life = 0. 311 Days (12-hr day; 1. 5E6 OH/cm3)Half-Life = 3. 727 HrsOzone Reaction: OVERALL Ozone Rate Constant = 1. 200000 E-17 cm3/molecule-secHalf-Life = 0. 955 Days (at 7E11 mol/cm3)Half-Life = 22. 920 HrsFraction sorbed to airborne particulates (phi): 1. 65E-006 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 8. 311Log Koc: 0. 920 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. 599 (BCF = 3. 97)log Kow used: 1. 69 (estimated)Volatilization from Water: Henry LC: 1. 31E-005 atm-m3/mole (estimated by Bond SAR Method)Half-Life from Model River: 45. 75 hours (1. 906 days)Half-Life from Model Lake : 583 hours (24. 29 days)Removal In Wastewater Treatment: Total removal: 2. 76 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 94 percentTotal to Air: 0. 73 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 762 5. 62 1000 Water 36 360 1000 Soil 63. 2 720 1000 Sediment 0. 0961 3. 24e+003 0 Persistence Time: 374 hr

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