

Dipropylamine $C_6H_{15}N$ structure



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Contents

- Retention Index (Normal Alkane):

Molecular
Formula $C_6H_{15}N$

Average mass 101. 190 Da

Density $0.7 \pm 0.1 \text{ g/cm}^3$

Boiling Point $108.8 \pm 0.0 \text{ }^\circ\text{C}$ at
760 mmHg

Flash Point $3.9 \pm 0.0 \text{ }^\circ\text{C}$

Molar
Refractivity $33.4 \pm 0.3 \text{ cm}^3$

Polarizability $13.3 \pm 0.5 \cdot 10^{-24}$
 cm^3

Surface
Tension $23.0 \pm 3.0 \text{ dyne/cm}$

Molar Volume $136.4 \pm 3.0 \text{ cm}^3$

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

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

- **Experimental Melting Point:**

-63 °CCTCID0930

-40 °COxford University

Chemical Safety Data

(No longer

updated)More details

-40 °CJean-Claude

Bradley Open Melting

Point Dataset16029

-63 °CJean-Claude

Bradley Open Melting

Point Dataset13348,

20116, 6950

-63 °CAIfa

AesarL15808

-63 °CSynQuest3131-1-

18

-63

°CLabNetworkLN00225

878

-63

°CFooDBFDB003929

- **Experimental Boiling Point:**

108-110 °COxford

University Chemical

Safety Data (No longer

updated)More details

109-110 °CAIfa

AesarL15808

105-110

°CSynQuest3131-1-18

105-110 °C

(Literature)LabNetwork

LN00225878

- **Experimental Flash Point:**

7 °COxford University

Chemical Safety Data

(No longer

updated)More details

7 °CAlfa Aesar

7 °F (-13. 8889 °C)Alfa

AesarL15808

7 °CSynQuest3131-1-

18

7

°CLabNetworkLN00225

878

- **Experimental Gravity:**

20 g/mLMerck Millipore1109

20 g/IMerck Millipore1109,

803548

0. 738 g/mLAlfa AesarL15808

0. 74 g/mLSynQuest3131-1-

18

- **Experimental Refraction Index:**

1. 405Alfa

AesarL15808

- Predicted Physico-chemical Properties

- **Predicted Melting Point:**

- 63 °CTCI

- 63

- °CTCID0930

- Miscellaneous

- **Appearance:**

- colourless liquidOxford

- University Chemical

- Safety Data (No longer

- updated)More details

- **Stability:**

- Stable. Highly

- flammable.

- Incompatible with

- strongoxidizing agents.

- Oxford University

- Chemical Safety Data

- (No longer

- updated)More details

- **Toxicity:**

- ORL-RAT LD50 300 mg

kg-1, SKN-RBT LD50

925 mg kg-1Oxford

University Chemical

Safety Data (No longer

updated)More details

- **Safety:**

1/2-16-26-36/37/39-

45Alfa AesarL15808

11-20/21/22-35Alfa

AesarL15808

16-26-36/37/39-45Alfa

AesarL15808

3Alfa AesarL15808

CORROSIVE /

FLAMMABLE /

HARMFULAlfa

AesarL15808

DangerAlfa

AesarL15808

H225-H314-H302-

H312-H332Alfa

AesarL15808

Highly

Flammable/Corrosive/H

armful/Lachrymatory/H

ygroscopicSynQuest31

31-1-18

P210-P260-

P303+P361+P353-

P305+P351+P338-

P405-P501aAlfa

AesarL15808

Safety glasses, gloves

(rubber), good

ventilation.

Removesources of

ignition from the

working area. Oxford

University Chemical

Safety Data (No longer

updated)More details

- Gas Chromatography

- **Retention Index (Kovats):**

816 (estimated with
error: 83)NIST
Spectramainlib_233533
, replib_228163,
replib_290912

750 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 3 m;
Column type: Packed;
Start T: 180 C; CAS no:
142847; Active phase:
PMS-100; Carrier gas:
He; Substrate: Celite
545 (44-60 mesh);
Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
pollyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-
63.)NIST Spectranist ri

752 (Program type:
Isothermal; Col... (show
more)umn class:
Standard non-polar;
Column length: 3 m;
Column type: Packed;
Start T: 130 C; CAS no:
142847; Active phase:
PMS-100; Carrier gas:
He; Substrate: Celite
545 (44-60 mesh);
Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and

pollyfunctional amines.

VII. Retention indices of

amines in some polar

and unpolar stationary

phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-63.,

Program type:

Isothermal; Col... (show

more)umn class:

Standard non-polar;

Column length: 3 m;

Column type: Packed;

Start T: 150 C; CAS no:

142847; Active phase:

PMS-100; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska,

M.; Golender, L., Gas-

liquid chromatography

of some aliphatic and

heterocyclic mono- and

pollyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-
63.)NIST Spectranist ri

742. 6 (Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 3. 3 m;
Column type: Packed;
Start T: 130 C; CAS no:
142847; Active phase:
C78, Branched paraffin;
Carrier gas: He; Data
type: Kovats RI;
Authors: Dallos, A.;
Sisak, A.; Kulcsar, Z.;
Kovats, E., Pair-wise
interactions by gas
chromatography VII.
Interaction free
enthalpies of solutes

with secondary alcohol groups, J. Chromatogr. A, 904, 2000, 211-242.,
Program type: Isothermal; Col... (show more)umn class: Semi-standard non-polar; Column length: 3. 3 m; Column type: Packed; Start T: 130 C; CAS no: 142847; Active phase: C78, Branched paraffin; Substrate: Chromosorb G HP; Data type: Kovats RI; Authors: Reddy, K. S.; Dutoit, J.-Cl.; Kovats, E. sz., Pair-wise interactions by gas chromatography. I. Interaction free enthalpies of solutes with non-associated primary alcohol groups, J. Chromatogr., 609, 1992, 229-259.)NIST

Spectranist ri

744 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 3. 7 m;

Column type: Packed;

Start T: 130 C; CAS no:

142847; Active phase:

Apolane; Data type:

Kovats RI; Authors:

Dutoit, J., Gas

chromatographic

retention behaviour of

some solutes on

structurally similar

polar and non-polar

stationary phases, J.

Chromatogr., 555,

1991, 191-204.)NIST

Spectranist ri

746 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;
Column length: 2. 26
m; Column type:
Packed; Start T: 130 C;
CAS no: 142847; Active
phase: Apiezon L;
Substrate: Teflon-
Haloport; Data type:
Kovats RI; Authors:
Landault, C.; Guiochon,
G., Separation des
amines par
chromatographie gaz-
liquide en utilisant le
teflon comme support,
J. Chromatogr., 13,
1964, 327-336.,
Program type:
Isothermal; Col... (show
more)umn class: Semi-
standard non-polar;
Column length: 2. 7 m;
Column type: Packed;
Start T: 100 C; CAS no:
142847; Active phase:
Apiezon L; Carrier gas:

N2; Substrate:

Chromosorb GAW; Data

type: Kovats RI;

Authors: Golovnya, R.

V.; Zhuravleva, N. L.;

Svetlova, N. I.;

Grigor'eva, D. N., Gas-

chromatographic

separation of

secondary normal

aliphatic amines, J.

Anal. Chem. USSR

(Engl. Transl.), 35(10),

1980, 1280-1285, In

original 1976-1981.,

Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column length: 2. 7 m;

Column type: Packed;

Start T: 100 C; CAS no:

142847; Active phase:

Apiezon L; Substrate:

Chromosorb G AW (80-

100 mesh); Data type:

Kovats RI; Authors:

Golovnya, R. V.;

Zhuravleva, I. L.;

Svetlova, I.; Terenina,

M. B.; Gutnik, S. B.,

Calculation of gas

chromatographic

retention indices of

secondary amines from

structural increments,

Zh. Anal. Khim., 37,

1982, 294-300.)NIST

Spectranist ri

748 (Program type:

Isothermal; Col... (show

more)umn class: Semi-

standard non-polar;

Column type: Packed;

Start T: 100 C; CAS no:

142847; Active phase:

Apiezon L; Data type:

Kovats RI; Authors:

Golovnya, R. V.;

Zhuravleva, I. L., Gas

Chromatographic

Method of Identification
of n-Aliphatic Amines
Through the Use of
Donor-Acceptor
Interaction with
Phosphate,
Chromatographia,
6(12), 1973, 508-
513.)NIST Spectranist ri

894 (Program type:
Isothermal; Col... (show
more)umn class:
Standard polar; Column
length: 3 m; Column
type: Packed; Start T:
200 C; CAS no:
142847; Active phase:
PEG-2000; Carrier gas:
He; Substrate: Celite
545 (44-60 mesh);
Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography

of some aliphatic and heterocyclic mono- and polyfunctional amines.

VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

900 (Program type:

Isothermal; Col... (show more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

179 C; CAS no:

142847; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska,

M.; Golender, L., Gas-

liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

901 (Program type:

Isothermal; Col... (show
more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

120 C; CAS no:

142847; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska,

M.; Golender, L., Gas-liquid chromatography of some aliphatic and heterocyclic mono- and pollyfunctional amines.

VII. Retention indices of amines in some polar and unpolar stationary phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

904 (Program type:

Isothermal; Col... (show more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

150 C; CAS no:

142847; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;

Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

905 (Program type:

Isothermal; Col... (show
more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

152 C; CAS no:

142847; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;

Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.

VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR

Zinat. Akad. Vestis Kim.

Ser., , 1973, 51-

63.)NIST Spectranist ri

910 (Program type:
Isothermal; Col... (show
more)umn class:

Standard polar; Column

length: 3 m; Column

type: Packed; Start T:

180 C; CAS no:

142847; Active phase:

PEG-2000; Carrier gas:

He; Substrate: Celite

545 (44-60 mesh);

Data type: Kovats RI;
Authors: Anderson, A.;
Jurel, S.; Shymanska,
M.; Golender, L., Gas-
liquid chromatography
of some aliphatic and
heterocyclic mono- and
polyfunctional amines.
VII. Retention indices of
amines in some polar
and unpolar stationary
phases, Latv. PSR
Zinat. Akad. Vestis Kim.
Ser., , 1973, 51-
63.)NIST Spectranist ri

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

748 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Capillary;
CAS no: 142847; Active
phase: Methyl Silicone;
Data type: Normal
alkane RI; Authors:

Chen, Y.; Feng, C.,
QSPR study on gas
chromatography
retention index of
some organic
pollutants, Comput.
Appl. Chem. (China),
24(10), 2007, 1404-
1408.)NIST Spectranist
ri

745 (Program type:
Ramp; Column cl...
(show more)ass:
Standard non-polar;
Column type: Capillary;
CAS no: 142847; Active
phase: Methyl Silicone;
Data type: Normal
alkane RI; Authors:
Zenkevich, I. G.,
Dependence of Gas
Chromatographic
Retention Indices on
Dynamics Molecular
Characteristics, Zh. Fiz.

Khim., 73(5), 1999,
905-910, In original
905-910.)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:	108.8±0.0 °C at 760 mmHg
Vapour Pressure:	25.5±0.2 mmHg at 25°C
Enthalpy of Vaporization:	33.5±0.0 kJ/mol
Flash Point:	3.9±0.0 °C
Index of Refraction:	1.405
Molar Refractivity:	33.4±0.3 cm ³
#H bond acceptors:	1
#H bond donors:	1
#Freely Rotating Bonds:	4
#Rule of 5 Violations:	0
ACD/LogP:	1.70

ACD/LogD (pH 5. 5):	-1. 38
ACD/BCF (pH 5. 5):	1. 00
ACD/KOC (pH 5. 5):	1. 00
ACD/LogD (pH 7. 4):	-1. 25
ACD/BCF (pH 7. 4):	1. 00
ACD/KOC (pH 7. 4):	1. 00
Polar Surface Area:	12 Å ²
Polarizability:	13. 3±0. 5 10 ⁻²⁴ cm ³
Surface Tension:	23. 0±3. 0 dyne/cm
Molar Volume:	136. 4±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. 79
Log Kow (Exper. database match) = 1. 67
Exper. Ref: Hansch, C et al. (1995)
Boiling Pt, Melting Pt, Vapor Pressure Estimations (MPBPWIN v1. 42):
Boiling Pt (deg C): 116. 83 (Adapted Stein & Brown method)
Melting Pt (deg C): -54. 28 (Mean or Weighted MP)
VP (mm Hg, 25 deg C): 25 (Mean VP of Antoine & Grain methods)
MP (exp database): -63 deg CBP (exp database): 109. 3 deg CVP (exp database): 2. 01E+01 mm Hg at 25 deg C
Water Solubility Estimate from Log Kow (WSKOW v1. 41): Water Solubility at 25 deg C (mg/L): 4. 429e+004
log Kow used: 1. 67 (expkow database)
no-melting pt equation used
Water Sol (Exper. database match) = 3. 51e+004 mg/L (25 deg C)
Exper. Ref: KUHNE, R ET AL. (1995)
Water Sol Estimate from Fragments: Wat Sol (v1. 01 est) = 39761 mg/L
Wat Sol (Exper. database match) = 35100. 00
Exper. Ref: KUHNE, R ET AL.

<https://assignbuster.com/dipropylamine-c6h15n-structure/>

(1995)ECOSAR Class Program (ECOSAR v0. 99h): Class(es) found: Aliphatic AminesHenry's Law Constant (25 deg C) [HENRYWIN v3. 10]: Bond Method : 5. 17E-005 atm-m³/moleGroup Method: 5. 23E-005 atm-m³/moleExper Database: 5. 10E-05 atm-m³/moleHenry's LC [VP/WSol estimate using EPI values]: 7. 516E-005 atm-m³/moleLog Octanol-Air Partition Coefficient (25 deg C) [KOAWIN v1. 10]: Log Kow used: 1. 67 (exp database)Log Kaw used: -2. 681 (exp database)Log Koa (KOAWIN v1. 10 estimate): 4. 351Log Koa (experimental database): 3. 590Probability of Rapid Biodegradation (BIOWIN v4. 10): Biowin1 (Linear Model) : 0. 8532Biowin2 (Non-Linear Model) : 0. 9359Expert Survey Biodegradation Results: Biowin3 (Ultimate Survey Model): 3. 0000 (weeks)Biowin4 (Primary Survey Model) : 3. 7450 (days-weeks)MITI Biodegradation Probability: Biowin5 (MITI Linear Model) : 0. 6429Biowin6 (MITI Non-Linear Model): 0. 7459Anaerobic Biodegradation Probability: Biowin7 (Anaerobic Linear Model): 0. 9582Ready 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): 2. 68E+003 Pa (20. 1 mm Hg)Log Koa (Exp database): 3. 590Kp (particle/gas partition coef. (m³/ug)): Mackay model : 1. 12E-009 Octanol/air (Koa) model: 9. 55E-010 Fraction sorbed to airborne particulates (phi): Junge-Pankow model : 4. 04E-008 Mackay model : 8. 96E-008 Octanol/air (Koa) model: 7. 64E-008 Atmospheric Oxidation (25 deg C) [AopWin v1. 92]: Hydroxyl Radicals Reaction: OVERALL OH Rate Constant = 87. 0003 E-12 cm³/mole-secHalf-Life = 0. 123 Days (12-hr day; 1. 5E6 OH/cm³)Half-Life = 1. 475 HrsOzone Reaction: No Ozone Reaction EstimationFraction sorbed to airborne particulates (phi): 6. 5E-008 (Junge, Mackay)Note: the sorbed fraction may be resistant to atmospheric oxidationSoil Adsorption Coefficient (PCKOCWIN v1. 66): Koc : 155. 1Log Koc: 2. 191 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. 586 (BCF = 3. 854)log Kow used: 1. 67 (expkow database)Volatilization from Water: Henry LC: 5. 1E-005 atm-m³/mole (Henry experimental database)Half-Life from Model River: 12. 57 hoursHalf-Life from Model Lake : 221. 5 hours (9. 23 days)Removal In Wastewater Treatment: Total removal: 4. 65 percentTotal biodegradation: 0. 09 percentTotal sludge adsorption: 1. 90 percentTotal to Air: 2. 66 percent(using 10000 hr Bio P, A, S)Level III Fugacity Model: Mass Amount Half-Life Emissions(percent) (hr) (kg/hr)Air 0. 567 2. 95 1000 Water 36. 6 360 1000 Soil 62. 7 720 1000 Sediment 0. 0965 3. 24e+003 0 Persistence Time: 326 hr

Click to predict properties on the Chemicalize site

- 1-Click Docking
- 1-Click Scaffold Hop