1-Hexadecanol

Other names:

1-Cetanol
1-Hexadecyl alcohol
1-Hexanedecanol
1-Hydroxyhexadecane
19141-82-3
Adol 52
Adol 52 NF
Adol 520
Adol 54
Alcohol c-16
Aldol 54
Alfol 16
Alfol 16RD
Atalco C
CO-1670
CO-1695
Cachalot C-50
Cachalot C-50 NF
Cachalot C-51
Cachalot C-52
Cetaffine
Cetal
Cetalol CA
Cetanol
Cetyl alcohol
Cetyl alcohol NF
Cetylic alcohol
Cetylol
Crodacol C
Crodacol C70
Crodacol C95 NF
Crodacol-CAS
Crodacol-CAT
Dytol F-11
ETHAL
Elfacos C
Epal 16
Epal 16NF
Ethol
Fancol CA

Hexadecan-1-ol
Hexadecanol
Hexadecyl alcohol
Hyfatol 16
Hyfatol 16-95
Kalcol 6098
Lanette 16
Lanol C
Laurex 16
Lipocol C
Lorol 24
Lorol C16
LorolL 24
Loxanol K
Loxanol K extra
Loxanwachs SK
N-CETYL ALCOHOL
N-HEXADECYL ALCOHOL
Palmitic alcohol
Palmityl alcohol
Philcohol 1600
Product 308
Rita CA
Siponol CC
Siponol wax-A
n-1-Hexadecanol
n-Hexadecan-1-ol
n-Hexadecanol

Inchi: InChI=1S/C16H34O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h17H,2-16H2,1H3
InchiKey: BXWNKGSJHAJOGX-UHFFFAOYSA-N
Formula: C16H34O
SMILES: CCCCCCCCCCCCCCCCO
Mol. weight [g/mol]: 242.44
CAS: 36653-82-4

Physical Properties

Property code	Value	Unit	Source
af	1.0180		KDB
chs	-10510.00 ± 8.00	kJ/mol	NIST Webbook

chs	-10471.90 ± 3.80	kJ/mol	NIST Webbook
chs	-10486.30 ± 1.70	kJ/mol	NIST Webbook
chs	-10468.90 ± 0.70	kJ/mol	NIST Webbook
gf	-52.98	kJ/mol	Joback Method
hf	-513.70	kJ/mol	NIST Webbook
hf	-517.50 ± 3.20	kJ/mol	NIST Webbook
hf	-516.80	kJ/mol	NIST Webbook
hfs	-687.10 ± 2.00	kJ/mol	NIST Webbook
hfs	-686.40 ± 0.40	kJ/mol	NIST Webbook
hfs	-683.30 ± 3.80	kJ/mol	NIST Webbook
hfus	54.79	kJ/mol	The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect
hfus	56.40	kJ/mol	Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry
hfus	107.70	kJ/mol	Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography
hsub	169.60	kJ/mol	NIST Webbook
hsub	169.50 ± 2.50	kJ/mol	NIST Webbook
hsub	169.50 ± 2.10	kJ/mol	NIST Webbook
hsub	167.00 ± 2.00	kJ/mol	NIST Webbook
hvap	108.80	kJ/mol	NIST Webbook
hvap	112.50	kJ/mol	NIST Webbook
hvap	107.70 ± 1.20	kJ/mol	NIST Webbook
log10ws	-7.26		Aqueous Solubility Prediction Method
log10ws	-7.00		Estimated Solubility Method
logp	5.460		Crippen Method
mcvol	242.170	ml/mol	McGowan Method
pc	1610.00	kPa	KDB
rinpol	1878.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1882.00		NIST Webbook

rinpol	1879.00	NIST Webbook
rinpol	1879.00	NIST Webbook
rinpol	1882.00	NIST Webbook
rinpol	1879.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1900.00	NIST Webbook
rinpol	1864.00	NIST Webbook
rinpol	1882.00	NIST Webbook
rinpol	1881.00	NIST Webbook
rinpol	1882.00	NIST Webbook
rinpol	1864.00	NIST Webbook
rinpol	1852.00	NIST Webbook
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rinpol	1856.00	NIST Webbook
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rinpol	1883.90	NIST Webbook
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rinpol	1881.00	NIST Webbook
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rinpol	1879.00	NIST Webbook
rinpol	1865.00	NIST Webbook
rinpol	1870.00	NIST Webbook
rinpol	1879.00	NIST Webbook
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rinpol	1882.00	NIST Webbook
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rinpol	1860.00	NIST Webbook
rinpol	1883.50	NIST Webbook
rinpol	1877.00	NIST Webbook
rinpol	1879.00	NIST Webbook
rinpol	1886.00	NIST Webbook
rinpol	1875.00	NIST Webbook
rinpol	1881.00	NIST Webbook
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rinpol	1872.00	NIST Webbook
rinpol	1890.00	NIST Webbook
rinpol	1884.00	NIST Webbook
rinpol	1885.00	NIST Webbook
rinpol	1894.00	NIST Webbook
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rinpol	312.09	NIST Webbook

rinpol	315.14	NIST Webbook
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ripol	2367.00	NIST Webbook
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ripol	2365.00	NIST Webbook
ripol	2400.00	NIST Webbook
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ripol	2386.00		NIST Webbook
ripol	2387.00		NIST Webbook
ripol	2383.00		NIST Webbook
ripol	2378.00		NIST Webbook
ripol	2393.00		NIST Webbook
ripol	2377.00		NIST Webbook
ripol	2376.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2380.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2384.00		NIST Webbook
ripol	2332.00		NIST Webbook
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ripol	2352.00		NIST Webbook
ripol	2342.00		NIST Webbook
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ripol	2365.00		NIST Webbook
ripol	2362.00		NIST Webbook
ripol	2352.00		NIST Webbook
ripol	2370.00		NIST Webbook
sg	853.00 ± 17.00	J/mol×K	NIST Webbook
ss	451.90	J/mol×K	NIST Webbook

tb	607.00	K	KDB
tb	613.15 ± 5.00	K	NIST Webbook
tc	770.00	K	KDB
tf	322.40	K	KDB
tf	322.80	K	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tf	324.23	K	Aqueous Solubility Prediction Method
tf	322.20	K	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
tf	322.91	K	Thermodynamics of organic mixtures containing amines. VIII. Systems with quinoline
tf	321.15	K	The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect
tf	322.20	K	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tf	323.51	K	Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry
tt	322.25 ± 0.06	K	NIST Webbook
tt	321.47 ± 0.10	K	NIST Webbook
tt	322.65 ± 0.50	K	NIST Webbook
tt	322.46 ± 0.05	K	NIST Webbook
tt	318.32 ± 0.30	K	NIST Webbook
tt	318.90 ± 0.30	K	NIST Webbook
tt	322.24 ± 0.06	K	NIST Webbook
vc	0.951	m3/kmol	KDB
zc	0.2390290		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	784.28	J/mol×K	817.45	Joback Method
cpg	709.54	J/mol×K	684.29	Joback Method
cpg	725.79	J/mol×K	710.92	Joback Method
cpg	741.37	J/mol×K	737.55	Joback Method
cpg	756.29	J/mol×K	764.18	Joback Method
cpg	770.59	J/mol×K	790.82	Joback Method
cpg	692.59	J/mol×K	657.66	Joback Method
cpl	618.20	J/mol×K	333.15	NIST Webbook
cpl	524.00	J/mol×K	323.00	NIST Webbook
cps	441.24	J/mol×K	290.00	NIST Webbook
cps	422.00	J/mol×K	298.15	NIST Webbook
dvisc	0.0018458	Pa×s	385.36	Joback Method
dvisc	0.0005925	Pa×s	439.82	Joback Method
dvisc	0.0002443	Pa×s	494.28	Joback Method
dvisc	0.0083589	Pa×s	330.90	Joback Method
dvisc	0.0000671	Pa×s	603.20	Joback Method
dvisc	0.0001201	Pa×s	548.74	Joback Method
dvisc	0.0000413	Pa×s	657.66	Joback Method
hfust	34.73	kJ/mol	320.00	NIST Webbook
hfust	57.70	kJ/mol	225.00	NIST Webbook
hfust	33.10	kJ/mol	321.60	NIST Webbook
hfust	33.97	kJ/mol	322.90	NIST Webbook
hsubt	167.40 ± 2.10	kJ/mol	314.00	NIST Webbook
hvapt	68.90	kJ/mol	539.00	NIST Webbook
hvapt	88.20	kJ/mol	403.00	NIST Webbook
hvapt	100.40	kJ/mol	345.00	NIST Webbook
hvapt	83.20	kJ/mol	451.00	NIST Webbook
hvapt	73.35	kJ/mol	617.20	KDB
hvapt	109.50	kJ/mol	329.00	NIST Webbook
hvapt	77.30	kJ/mol	521.50	NIST Webbook
hvapt	78.80	kJ/mol	440.50	NIST Webbook
hvapt	112.30	kJ/mol	349.50	NIST Webbook
hvapt	109.40	kJ/mol	329.00	NIST Webbook
sfust	108.50	J/mol×K	320.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbp	465.70	K	2.02	Vapor-liquid equilibria of monoacylglicerol + monoacylglicerol or alcohol or fatty acid at subatmospheric pressures
tbrp	453.20	K	1.30	NIST Webbook
tfp	322.20	K	100.00	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tfp	327.30	K	20000.00	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tfp	332.40	K	40000.00	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol
tfp	337.60	K	60000.00	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol

tfp	342.70	K	80000.00	High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol

Sources

High Pressure Solid-Liquid Equilibrium of Fatty Alcohols Binary Systems from 1-Dodecanol, 1-Tetradecanol, 1-Hexadecanol, and 1-Octadecanol:	https://www.doi.org/10.1021/acs.jced.5b00330
Thermodynamics of organic mixtures containing amines, VIII. Systems with quinoline:	https://www.doi.org/10.1016/j.jct.2008.03.015
Vapor-liquid equilibria of monoacylglicerol + monoacylglicerol or alcohol or fatty acid at subatmospheric pressures:	https://www.doi.org/10.1016/j.fluid.2017.08.013
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
Vapor-Liquid Equilibria of Binary Systems with Long-Chain Organic Compounds (Fatty Alcohol, Fatty Ester, Acylglycerol, and n-Paraffin) at Subatmospheric Pressures:	https://www.doi.org/10.1021/acs.jced.8b00168
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=856
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C36653824&Units=SI
Aqueous Solubility Prediction Method:	http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa
Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanediol at atmospheric and high pressure:	https://www.doi.org/10.1016/j.fluid.2006.02.001
Solid-Liquid Equilibrium of Binary Systems Containing Fatty Acids and Fatty Alcohols Using Differential Scanning Calorimetry:	https://www.doi.org/10.1021/acs.jced.8b01006
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Estimated Solubility Method:	http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt
Evaluation of the Vaporization, Fusion, and Sublimation Enthalpies of the 1-Alkanols: The Vaporization Enthalpy of 1-, 6-, 7-, and 9-Heptadecanol, 1-Octadecanol, 1-Eicosanol, 1-Docosanol, 1-Hexacosanol, and Cholesterol at T) 298.15 K by Correlation Gas Chromatography:	https://www.doi.org/10.1021/je0503857
KDB:	https://www.cheric.org/files/research/kdb/mol/mol856.mol
The manufacture of organic carbonate-poly(methyl ethylacrylate) nanowebs with thermal buffering effect:	https://www.doi.org/10.1016/j.tca.2017.10.003

Legend

af:	Acentric Factor
chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
cpl:	Liquid phase heat capacity
cps:	Solid phase heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions

hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation at standard conditions
hsubt:	Enthalpy of sublimation at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
sfust:	Entropy of fusion at a given temperature
sg:	Molar entropy at standard conditions
ss:	Solid phase molar entropy at standard conditions
tb:	Normal Boiling Point Temperature
tbp:	Boiling point at given pressure
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
tt:	Triple Point Temperature
vc:	Critical Volume
zc:	Critical Compressibility