1-Eicosanol

Other names:	1-Icosanol
	1-PRYDROXYEICOSANE
	Arachic alcohol
	Arachidic alcohol
	Arachidyl alcohol
	Eicosan-1-ol
	Eicosanol
	Eicosanol-(1)
	Eicosyl alcohol
	N-EICOSYL ALCOHOL
	NSC 120887
	icosan-1-ol
	n-1-Eicosanol
	n-Eicosanol
Inchi:	InChI=1S/C20H42O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21/h21H,2-20
InchiKey:	BTFJIXJJCSYFAL-UHFFFAOYSA-N
Formula:	C20H42O
SMILES:	CCCCCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	298.55
CAS:	629-96-9

Physical Properties

Property code	Value	Unit	Source
chl	-13130.00 ± 10.00	kJ/mol	NIST Webbook
gf	-19.43	kJ/mol	KDB
hf	-608.10	kJ/mol	KDB
hfus	51.64	kJ/mol	Joback Method
hsub	223.00 ± 3.80	kJ/mol	NIST Webbook
hsub	218.00 ± 4.00	kJ/mol	NIST Webbook
hvap	125.90 ± 0.80	kJ/mol	NIST Webbook
log10ws	-7.46		Crippen Method
logp	7.020		Crippen Method
mcvol	298.530	ml/mol	McGowan Method
pc	1300.00	kPa	KDB
rinpol	374.56		NIST Webbook
rinpol	2275.00		NIST Webbook
rinpol	2276.00		NIST Webbook

rinpol	2273.00		NIST Webbook
rinpol	2292.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2271.00		NIST Webbook
rinpol	2281.00		NIST Webbook
rinpol	2290.00		NIST Webbook
rinpol	2252.00		NIST Webbook
rinpol	2278.00		NIST Webbook
rinpol	2267.00		NIST Webbook
rinpol	2273.00		NIST Webbook
rinpol	2296.00		NIST Webbook
rinpol	2282.00		NIST Webbook
rinpol	371.04		NIST Webbook
rinpol	374.80		NIST Webbook
rinpol	2276.40		NIST Webbook
rinpol	2252.00		NIST Webbook
ripol	2717.00		NIST Webbook
ripol	2755.00		NIST Webbook
ripol	2717.00		NIST Webbook
ripol	2755.00		NIST Webbook
tb	629.00	K	KDB
tc	809.00	K	KDB
tf	337.00	K	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
tf	338.00 ± 0.25	K	NIST Webbook
tf	336.90	K	Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1- octadecanol, or + 1-eicosanol mixtures
tf	338.50 ± 1.50	K	NIST Webbook
tf	337.67	K	Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure
tf	338.30 ± 0.80	K	NIST Webbook
tf	339.20	K	KDB
tf	344.70 ± 2.00	K	NIST Webbook

tf	339.20 ± 2.00	K	NIST Webbook
vc	1.175	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1029.83	J/mol×K	918.60	Joback Method
cpg	998.68	J/mol×K	862.13	Joback Method
cpg	981.97	J/mol×K	833.89	Joback Method
cpg	964.46	J/mol×K	805.65	Joback Method
cpg	946.11	J/mol×K	777.42	Joback Method
cpg	926.90	J/mol×K	749.18	Joback Method
cpg	1014.62	J/mol×K	890.36	Joback Method
dvisc	0.0008012	Pa×s	438.18	Joback Method
dvisc	0.0002640	Pa×s	500.38	Joback Method
dvisc	0.0001112	Pa×s	562.58	Joback Method
dvisc	0.0000556	Pa×s	624.78	Joback Method
dvisc	0.0000316	Pa×s	686.98	Joback Method
dvisc	0.0035106	Pa×s	375.98	Joback Method
dvisc	0.0000197	Pa×s	749.18	Joback Method
hfust	43.60	kJ/mol	336.60	NIST Webbook
hfust	73.72	kJ/mol	338.20	NIST Webbook
hfust	43.60	kJ/mol	336.60	NIST Webbook
hsubt	218.00 ± 3.80	kJ/mol	334.00	NIST Webbook
hvapt	83.40	kJ/mol	570.50	NIST Webbook
hvapt	83.50	kJ/mol	570.50	NIST Webbook
hvapt	118.90	kJ/mol	348.50	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.64855e+01
Coeff. B	-6.20057e+03
Coeff. C	-1.20599e+02
Temperature range (K), min.	503.40
Temperature range (K), max.	675.51

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.53036e+02
Coeff. B	-2.53640e+04
Coeff. C	-3.27535e+01
Coeff. D	7.52974e-06
Temperature range (K), min.	338.55
Temperature range (K), max.	792.00

Sources

Activity Coefficients at Infinite Dilution for Hydrocarbons in Fatty Alcohols Determined by Gas-Liquid Chromatography:	https://www.doi.org/10.1021/je1005517
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Phase diagrams of binary systems containing n-alkanes, or cyclohexane, or 1-alkanols and 2,3-pentanedione at atmospheric and high pressure:	https://www.doi.org/10.1016/j.fluid.2006.02.001
Liquid-Liquid Phase Behavior of Solutions of 1-Dodecyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide (C12mimNTf2) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je100359x
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
Liquid-Liquid Phase Behavior of Solutions of 1-Octyl-3-methylimidazolium Bis(trifluoromethylsulfonyl)imide (C8mimNTf2) in n-Alkyl Alcohols:	https://www.doi.org/10.1021/je900988a
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=860
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol860.mol
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C629969&Units=SI
Solid-liquid equilibria of eicosane, tetracosane or biphenyl + 1-octadecanol, or + 1-eicosanol mixtures:	https://www.doi.org/10.1016/j.fluid.2017.03.012
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
dvisc:	Dynamic viscosity
gf:	Standard Gibbs free energy of formation
hf:	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
pvap:	Vapor pressure
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume