n-Heptadecanol-1

Other names:	1-HEPTADECANOL
	1-HYDROXYHEPTADECANE
	Heptadecan-1-ol
	Heptadecanol
	Heptadecyl alcohol
	N-HEPTADECYL ALCOHOL
Inchi:	InChI=1S/C17H36O/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18/h18H,2-17H2,1H3
InchiKey:	GOQYKNQRPGWPLP-UHFFFAOYSA-N
Formula:	C17H36O
SMILES:	CCCCCCCCCCCCCCCCCO
Mol. weight [g/mol]:	256.47
CAS:	1454-85-9

Physical Properties

Property code	Value	Unit	Source
gf	-44.67	kJ/mol	KDB
hf	-546.30	kJ/mol	KDB
hfus	39.40	kJ/mol	Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlationos for the heat capacity and the entropy of liquid n-alcohols
hvap	112.50 ± 0.50	kJ/mol	NIST Webbook
log10ws	-6.20		Crippen Method
logp	5.850		Crippen Method
mcvol	256.260	ml/mol	McGowan Method
pc	1500.00	kPa	KDB
rinpol	1986.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1949.00		NIST Webbook
rinpol	1982.00		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1960.00		NIST Webbook

rinpol	1968.00		NIST Webbook
rinpol	1993.10		NIST Webbook
rinpol	1960.00		NIST Webbook
rinpol	1975.00		NIST Webbook
rinpol	1941.00		NIST Webbook
rinpol	1993.00		NIST Webbook
rinpol	1974.00		NIST Webbook
rinpol	1979.00		NIST Webbook
ripol	2445.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2498.00		NIST Webbook
ripol	2451.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2496.00		NIST Webbook
ripol	2524.00		NIST Webbook
ripol	2482.00		NIST Webbook
ripol	2498.00		NIST Webbook
tb	606.00	K	KDB
tb	581.20	K	NIST Webbook
tc	780.00	K	KDB
tf	327.15 ± 0.40	K	NIST Webbook
tf	325.30	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	326.90	K	KDB
vc	1.006	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	843.94	J/mol×K	841.88	Joback Method
cpg	783.74	J/mol×K	734.32	Joback Method
cpg	799.79	J/mol×K	761.21	Joback Method
cpg	815.16	J/mol×K	788.10	Joback Method

cpg	829.86	J/mol×K	814.99	Joback Method
cpg	749.49	J/mol×K	680.54	Joback Method
cpg	766.98	J/mol×K	707.43	Joback Method
cpl	649.60	J/mol×K	333.15	NIST Webbook
dvisc	0.0000343	Pa×s	680.54	Joback Method
dvisc	0.0000990	Pa×s	567.75	Joback Method
dvisc	0.0002005	Pa×s	511.36	Joback Method
dvisc	0.0004834	Pa×s	454.96	Joback Method
dvisc	0.0014953	Pa×s	398.56	Joback Method
dvisc	0.0000556	Pa×s	624.14	Joback Method
dvisc	0.0067109	Pa×s	342.17	Joback Method
hfust	37.00	kJ/mol	326.60	NIST Webbook
hfust	63.06	kJ/mol	327.30	NIST Webbook
hfust	37.00	kJ/mol	326.60	NIST Webbook
hvapt	78.30	kJ/mol	540.00	NIST Webbook
hvapt	75.90	kJ/mol	548.00	NIST Webbook
hvapt	60.67	kJ/mol	597.00	KDB
rhol	848.00	kg/m3	327.00	KDB

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.61609e+01
Coeff. B	-5.70883e+03
Coeff. C	-1.08270e+02
Temperature range (K), min.	467.92
Temperature range (K), max.	634.46

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	2.32218e+02
Coeff. B	-2.23722e+04
Coeff. C	-3.02228e+01
Coeff. D	8.42167e-06
Temperature range (K), min.	327.05
Temperature range (K), max.	770.00

Sources

Heat capacities and derived thermodynamic functions of 1-dodecanol and 1-tridecanol between 10 K and 370 K and heat capacities of 1-pentadecanol and 1-heptadecanol between 300 K and 380 K and correlations for the heat capacity and the enthalpy of liquid n-alcohols:	https://www.doi.org/10.1021/je0255240
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
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
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=857
KDB:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=857
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1454859&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

cpg:	Ideal gas heat capacity
cpl:	Liquid phase 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
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
rhol:	Liquid Density
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