Hexadecane, 1-chloro-

Other names:	1-Chlorohexadecane
	CETYL CHLORIDE
	Hexadecyl chloride
	N-HEXADECYL CHLORIDE
	Palmityl chloride
Inchi:	InChI=1S/C16H33Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17/h2-16H2,1H3
InchiKey:	CLWAXFZCVYJLLM-UHFFFAOYSA-N
Formula:	C16H33Cl
SMILES:	CCCCCCCCCCCCCCCCCl
Mol. weight [g/mol]:	260.89
CAS:	4860-03-1

Physical Properties

Property code	Value	Unit	Source
gf	71.91	kJ/mol	Joback Method
hf	-389.31	kJ/mol	Joback Method
hfus	41.39	kJ/mol	Joback Method
hvap	97.90	kJ/mol	NIST Webbook
hvap	96.40 ± 0.90	kJ/mol	NIST Webbook
hvap	91.80 ± 1.10	kJ/mol	NIST Webbook
hvap	91.80	kJ/mol	NIST Webbook
hvap	91.80 ± 1.10	kJ/mol	NIST Webbook
log10ws	-6.67		Crippen Method
logp	6.707		Crippen Method
mcvol	248.540	ml/mol	McGowan Method
pc	1283.75	kPa	Joback Method
rinpol	1873.00		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	277.60		NIST Webbook
rinpol	1873.00		NIST Webbook
rinpol	277.60		NIST Webbook
rinpol	1861.00		NIST Webbook
rinpol	1871.00		NIST Webbook
ripol	2078.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2094.00		NIST Webbook

ripol	2078.00		NIST Webbook
ripol	2099.00		NIST Webbook
ripol	2104.00		NIST Webbook
ripol	2094.00		NIST Webbook
tb	595.20	K	NIST Webbook
tb	468.15	K	KDB
tc	766.68	K	Joback Method
tf	290.48	K	KDB
vc	0.981	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	650.15	J/mol×K	602.91	Joback Method
cpg	668.61	J/mol×K	630.20	Joback Method
cpg	686.30	J/mol×K	657.50	Joback Method
cpg	703.26	J/mol×K	684.79	Joback Method
cpg	719.50	J/mol×K	712.09	Joback Method
cpg	735.05	J/mol×K	739.38	Joback Method
cpg	749.92	J/mol×K	766.68	Joback Method
dvisc	0.0039733	Pa×s	300.00	Joback Method
dvisc	0.0015295	Pa×s	350.49	Joback Method
dvisc	0.0007487	Pa×s	400.97	Joback Method
dvisc	0.0004300	Pa×s	451.45	Joback Method
dvisc	0.0002761	Pa×s	501.94	Joback Method
dvisc	0.0001923	Pa×s	552.42	Joback Method
dvisc	0.0001422	Pa×s	602.91	Joback Method
hvapt	73.30	kJ/mol	519.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	422.20	K	0.10	NIST Webbook

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.59946e+01
Coeff. B	-5.54330e+03
Coeff. C	-1.07880e+02
Temperature range (K), min.	460.80
Temperature range (K), max.	626.77

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.64572e+02
Coeff. B	-1.67676e+04
Coeff. C	-2.10675e+01
Coeff. D	7.73533e-06
Temperature range (K), min.	438.15
Temperature range (K), max.	600.15

Sources

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

KDB Vapor Pressure Data: https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=1656

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Joback Method: https://en.wikipedia.org/wiki/Joback_method

KDB: https://www.cheric.org/files/research/kdb/mol/mol1656.mol

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4860031&Units=SI

Legend

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
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
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume