Octadecane, 1-chloro-

Other names:	1-Chlorooctadecane
	Chlorooctadecane
	N-OCTADECYL CHLORIDE
	Octadecyl chloride
Inchi:	InChI=1S/C18H37Cl/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-18-19/h2-18H2,1H3
InchiKey:	VUQPJRPDRDVQMN-UHFFFAOYSA-N
Formula:	C18H37Cl
SMILES:	CCCCCCCCCCCCCCCCCCCl
Mol. weight [g/mol]:	288.94
CAS:	3386-33-2

Physical Properties

Property code	Value	Unit	Source
gf	88.75	kJ/mol	Joback Method
hf	-430.59	kJ/mol	Joback Method
hfus	46.57	kJ/mol	Joback Method
hvap	60.05	kJ/mol	Joback Method
log10ws	-7.51		Crippen Method
logp	7.487		Crippen Method
mcvol	276.720	ml/mol	McGowan Method
pc	1123.81	kPa	Joback Method
rinpol	2069.80		NIST Webbook
rinpol	2079.00		NIST Webbook
rinpol	346.70		NIST Webbook
rinpol	2070.00		NIST Webbook
ripol	2294.00		NIST Webbook
ripol	2312.00		NIST Webbook
ripol	2288.00		NIST Webbook
tb	292.65	K	KDB
tc	812.72	K	Joback Method
tf	292.65	K	KDB
vc	1.093	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	762.81	J/mol×K	648.67	Joback Method
cpg	782.14	J/mol×K	676.01	Joback Method
cpg	800.65	J/mol×K	703.35	Joback Method
cpg	818.38	J/mol×K	730.70	Joback Method
cpg	835.34	J/mol×K	758.04	Joback Method
cpg	851.56	J/mol×K	785.38	Joback Method
cpg	867.07	J/mol×K	812.72	Joback Method
dvisc	0.0033349	Pa×s	322.54	Joback Method
dvisc	0.0012601	Pa×s	376.89	Joback Method
dvisc	0.0006085	Pa×s	431.25	Joback Method
dvisc	0.0003459	Pa×s	485.61	Joback Method
dvisc	0.0002203	Pa×s	539.96	Joback Method
dvisc	0.0001524	Pa×s	594.32	Joback Method
dvisc	0.0001121	Pa×s	648.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.40282e+01
Coeff. B	-5.03151e+03
Coeff. C	-1.14942e+02
Temperature range (K), min.	481.12
Temperature range (K), max.	692.17

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.24085e+02
Coeff. B	-1.52071e+04
Coeff. C	-1.50336e+01
Coeff. D	4.43161e-06
Temperature range (K), min.	472.15

Temperature range (K), max.	673.15

Sources

KDB:	https://www.cheric.org/files/research/kdb/mol/mol1658.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3386332&Units=SI
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=1658
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

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
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