n-Tridecylcyclohexane

Other names:	Cyclohexane, tridecyl- TRIDECYLCYCLOHEXANE tridecane, 1-cyclohexyl-
Inchi:	InChI=1S/C19H38/c1-2-3-4-5-6-7-8-9-10-11-13-16-19-17-14-12-15-18-19/h19H,2-18H2,1
InchiKey:	DKRUJKKWJGNYQN-UHFFFAOYSA-N
Formula:	C19H38
SMILES:	CCCCCCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	266.50
CAS:	6006-33-3

Physical Properties

Property code	Value	Unit	Source
af	0.7000		KDB
chl	-12509.00 ± 2.80	kJ/mol	NIST Webbook
gf	133.55	kJ/mol	Joback Method
hf	-398.70 ± 3.10	kJ/mol	NIST Webbook
hfus	36.80	kJ/mol	Joback Method
hvap	94.50	kJ/mol	NIST Webbook
log10ws	-7.43		Crippen Method
logp	7.268		Crippen Method
mcvol	267.710	ml/mol	McGowan Method
pc	1240.00	kPa	KDB
rinpol	1949.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1918.00		NIST Webbook
rinpol	1950.00		NIST Webbook
tb	600.00 ± 3.00	K	NIST Webbook
tb	614.70	K	KDB
tc	783.40	K	KDB
tf	292.00	K	KDB
vc	1.032	m3/kmol	KDB
zc	0.1965580		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	883.55	J/mol×K	803.20	Joback Method
cpg	864.71	J/mol×K	773.29	Joback Method
cpg	844.86	J/mol×K	743.39	Joback Method
cpg	823.95	J/mol×K	713.48	Joback Method
cpg	801.95	J/mol×K	683.58	Joback Method
cpg	778.82	J/mol×K	653.67	Joback Method
cpg	901.40	J/mol×K	833.10	Joback Method
dvisc	0.0049003	Pa×s	311.27	Joback Method
dvisc	0.0001161	Pa×s	653.67	Joback Method
dvisc	0.0001608	Pa×s	596.60	Joback Method
dvisc	0.0002385	Pa×s	539.54	Joback Method
dvisc	0.0003884	Pa×s	482.47	Joback Method
dvisc	0.0007208	Pa×s	425.40	Joback Method
dvisc	0.0016200	Pa×s	368.34	Joback Method
hvapt	55.10	kJ/mol	614.70	KDB
hvapt	72.20	kJ/mol	562.50	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	286.90	K	100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	291.70	K	20000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	296.30	K	40200.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	300.70	K	60000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

tfp	304.90	K	80100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	309.10	K	100000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.54555e+01
Coeff. B	-5.14804e+03
Coeff. C	-1.24963e+02
Temperature range (K), min.	464.37
Temperature range (K), max.	632.46

Sources

The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes:	https://www.doi.org/10.1021/je600575r
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol603.mol
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C6006333&Units=SI

Legend

af:	Acentric Factor
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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
tfp:	Melting point
vc:	Critical Volume
zc:	Critical Compressibility