Cyclohexane, undecyl-

Other names:	1-cyclohexylundecane
	UNDECYLCYCLOHEXANE
	n-Undecylcyclohexane
	n-Undecylcylcohexane
	undecane, 1-cyclohexyl-
Inchi:	InChI=1S/C17H34/c1-2-3-4-5-6-7-8-9-11-14-17-15-12-10-13-16-17/h17H,2-16H2,1H3
InchiKey:	XQQVOBPJWHQXEN-UHFFFAOYSA-N
Formula:	C17H34
SMILES:	CCCCCCCCCCCC1CCCCC1
Mol. weight [g/mol]:	238.45
CAS:	54105-66-7

Physical Properties

Property code	Value	Unit	Source
af	0.6460		KDB
chl	-11191.50 ± 2.40	kJ/mol	NIST Webbook
gf	116.71	kJ/mol	Joback Method
hf	-357.40 ± 2.60	kJ/mol	NIST Webbook
hfus	31.62	kJ/mol	Joback Method
hvap	84.60	kJ/mol	NIST Webbook
log10ws	-6.59		Crippen Method
logp	6.488		Crippen Method
mcvol	239.530	ml/mol	McGowan Method
pc	1430.00	kPa	KDB
rinpol	1760.00		NIST Webbook
rinpol	1760.00		NIST Webbook
tb	586.30	K	KDB
tb	574.00 ± 4.00	K	NIST Webbook
tc	761.70	K	KDB
tf	279.00	K	KDB
vc	0.920	m3/kmol	KDB
zc	0.2078450		KDB

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	765.56	J/mol×K	759.55	Joback Method
cpg	746.98	J/mol×K	729.22	Joback Method
cpg	727.40	J/mol×K	698.89	Joback Method
cpg	706.79	J/mol×K	668.56	Joback Method
cpg	685.11	J/mol×K	638.24	Joback Method
cpg	662.34	J/mol×K	607.91	Joback Method
cpg	783.17	J/mol×K	789.87	Joback Method
dvisc	0.0059390	Pa×s	288.73	Joback Method
dvisc	0.0001466	Pa×s	607.91	Joback Method
dvisc	0.0002022	Pa×s	554.71	Joback Method
dvisc	0.0002983	Pa×s	501.52	Joback Method
dvisc	0.0004829	Pa×s	448.32	Joback Method
dvisc	0.0008899	Pa×s	395.12	Joback Method
dvisc	0.0019833	Pa×s	341.93	Joback Method
hvapt	52.05	kJ/mol	586.30	KDB
hvapt	67.00	kJ/mol	536.00	NIST Webbook

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tfp	272.40	K	100.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	276.80	K	20000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	281.30	K	40000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	285.70	K	60000.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes

tfp	289.90	K	80500.00	Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes
tfp	293.90	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	1.53758e+01
Coeff. B	-5.00915e+03
Coeff. C	-1.08357e+02
Temperature range (K), min.	440.35
Temperature range (K), max.	606.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.46191e+02
Coeff. B	-1.53860e+04
Coeff. C	-1.84191e+01
Coeff. D	6.02369e-06
Temperature range (K), min.	460.00
Temperature range (K), max.	642.00

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
KDB Vapor Pressure Data:	https://www.cheric.org/research/kdb/hcprop/showprop.php?cmpid=598
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
KDB:	https://www.cheric.org/files/research/kdb/mol/mol598.mol
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54105667&Units=SI
Solid-Liquid Equilibria under High Pressure of Eight Pure n-Alkylcyclohexanes:	https://www.doi.org/10.1021/je600575r

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
The Yaws Handbook of Vapor Pressure:	https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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

Latest version available from:

https://www.chemeo.com/cid/54-379-2/Cyclohexane-undecyl.pdf

Generated by Cheméo on 2024-04-24 16:43:03.69265223 +0000 UTC m=+16266232.613229541.

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.