Cyclopentane, hexyl-

Other names:	Hexylcyclopentane
	N-HEXYLCYCLOPENTANE
Inchi:	InChI=1S/C11H22/c1-2-3-4-5-8-11-9-6-7-10-11/h11H,2-10H2,1H3
InchiKey:	LKHGKBBAJAFMSQ-UHFFFAOYSA-N
Formula:	C11H22
SMILES:	CCCCCCC1CCCC1
Mol. weight [g/mol]:	154.29
CAS:	4457-00-5

Physical Properties

Property code	Value	Unit	Source
chl	-7263.40 ± 1.50	kJ/mol	NIST Webbook
gf	78.29	kJ/mol	Joback Method
hf	-209.50 ± 1.60	kJ/mol	NIST Webbook
hfus	18.18	kJ/mol	Joback Method
hvap	55.90	kJ/mol	NIST Webbook
ie	9.90 ± 0.03	eV	NIST Webbook
log10ws	-4.08		Crippen Method
logp	4.147		Crippen Method
mcvol	154.990	ml/mol	McGowan Method
pc	2280.59	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1138.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1133.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1136.00		NIST Webbook
rinpol	1132.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1134.00		NIST Webbook
rinpol	1141.00		NIST Webbook
rinpol	1137.00		NIST Webbook
rinpol	1137.90		NIST Webbook
rinpol	1135.00		NIST Webbook
rinpol	1136.00		NIST Webbook
ripol	1196.00		NIST Webbook

ripol	1200.00		NIST Webbook
ripol	1204.00		NIST Webbook
ripol	1208.00		NIST Webbook
ripol	1212.00		NIST Webbook
ripol	1188.00		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1196.20		NIST Webbook
ripol	1199.70		NIST Webbook
ripol	1204.40		NIST Webbook
ripol	1199.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1187.50		NIST Webbook
ripol	1192.00		NIST Webbook
ripol	1207.00		NIST Webbook
ripol	1208.50		NIST Webbook
ripol	1194.00		NIST Webbook
ripol	1212.40		NIST Webbook
tb	466.36	K	Joback Method
tc	653.79	K	Joback Method
tf	224.63	K	Joback Method
vc	0.593	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	346.42	J/mol×K	466.36	Joback Method
cpg	433.68	J/mol×K	622.55	Joback Method
cpg	417.92	J/mol×K	591.31	Joback Method
cpg	401.35	J/mol×K	560.08	Joback Method
cpg	383.93	J/mol×K	528.84	Joback Method
cpg	365.63	J/mol×K	497.60	Joback Method
cpg	448.64	J/mol×K	653.79	Joback Method
dvisc	0.0002968	Pa×s	466.36	Joback Method
dvisc	0.0003829	Pa×s	426.07	Joback Method
dvisc	0.0005211	Pa×s	385.78	Joback Method
dvisc	0.0007620	Pa×s	345.50	Joback Method
dvisc	0.0012318	Pa×s	305.21	Joback Method
dvisc	0.0023045	Pa×s	264.92	Joback Method
dvisc	0.0053976	Pa×s	224.63	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.56840e+01
Coeff. B	-4.34114e+03
Coeff. C	-7.35500e+01
Temperature range (K), min.	355.51
Temperature range (K), max.	492.07

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/T + C*ln(T) + D*T^2
Coeff. A	1.21252e+02
Coeff. B	-1.09839e+04
Coeff. C	-1.54782e+01
Coeff. D	8.22833e-06
Temperature range (K), min.	351.00
Temperature range (K), max.	507.15

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=590

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/mol590.mol

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C4457005&Units=SI

Legend

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
ie:	Ionization energy
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