3-Chlorohexane

Other names: Hexane, 3-chloro-
Inchi: InChI=1S/C6H13Cl/c1-3-5-6(7)4-2/h6H,3-5H2,1-2H3
InchiKey: BXSMMAVTEURRGG-UHFFFAOYSA-N
Formula: C6H13Cl
SMILES: CCCC(Cl)CC
Mol. weight [g/mol]: 120.62
CAS: 2346-81-8

Physical Properties

Property code	Value	Unit	Source
gf	-14.73	kJ/mol	Joback Method
hf	-188.19	kJ/mol	Joback Method
hfus	11.97	kJ/mol	Joback Method
hvap	32.95	kJ/mol	Joback Method
log10ws	-2.60		Crippen Method
logp	2.804		Crippen Method
mcvol	107.640	ml/mol	McGowan Method
pc	3009.03	kPa	Joback Method
rinpol	795.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	812.00		NIST Webbook
rinpol	801.00		NIST Webbook
ripol	967.00		NIST Webbook
ripol	982.00		NIST Webbook
ripol	965.00		NIST Webbook
ripol	974.00		NIST Webbook
tb	396.00 ± 5.00	K	NIST Webbook
tc	550.01	K	Joback Method
tf	172.30	K	Joback Method
vc	0.414	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	185.85	J/mol×K	373.67	Joback Method
cpg	196.56	J/mol×K	403.06	Joback Method
cpg	206.84	J/mol×K	432.45	Joback Method
cpg	216.72	J/mol×K	461.84	Joback Method
cpg	226.20	J/mol×K	491.23	Joback Method
cpg	235.29	J/mol×K	520.62	Joback Method
cpg	244.00	J/mol×K	550.01	Joback Method
dvisc	0.0084225	Pa×s	172.30	Joback Method
dvisc	0.0030184	Pa×s	205.86	Joback Method
dvisc	0.0014423	Pa×s	239.42	Joback Method
dvisc	0.0008264	Pa×s	272.99	Joback Method
dvisc	0.0005349	Pa×s	306.55	Joback Method
dvisc	0.0003773	Pa×s	340.11	Joback Method
dvisc	0.0002833	Pa×s	373.67	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.55088e+01
Coeff. B	-3.75415e+03
Coeff. C	-5.12800e+01
Temperature range (K), min.	297.92
Temperature range (K), max.	419.43

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C2346818&Units=SI

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

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

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

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