1,1-Dichlorohexane

Other names: Hexane, 1,1-dichloro
Inchi: InChI=1S/C6H12Cl2/c1-2-3-4-5-6(7)8/h6H,2-5H2,1H3
InchiKey: RQXXCWHCUOJQGR-UHFFFAOYSA-N
Formula: C6H12Cl2
SMILES: CCCCCC(Cl)Cl
Mol. weight [g/mol]: 155.06
CAS: 62017-16-7

Physical Properties

Property code	Value	Unit	Source
af	0.3723		Cheméo Relay (1.0)
gf	-26.66	kJ/mol	Joback Method
hf	-200.95	kJ/mol	Cheméo Relay (1.0)
hfus	16.17	kJ/mol	Joback Method
hvap	48.70	kJ/mol	NIST Webbook
ie	10.54	eV	Cheméo Relay (1.0)
log10ws	-3.74		Cheméo Relay (1.0)
logp	3.370		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2890.51	kPa	Joback Method
tb	433.94	K	Cheméo Relay (1.0)
tc	618.27	K	Cheméo Relay (1.0)
tf	192.48	K	Cheméo Relay (1.0)
vc	0.451	m3/kmol	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	212.27	J/mol×K	411.10	Joback Method
cpg	222.72	J/mol×K	441.81	Joback Method
cpg	232.70	J/mol×K	472.52	Joback Method
cpg	242.24	J/mol×K	503.23	Joback Method
cpg	251.35	J/mol×K	533.95	Joback Method
cpg	260.04	J/mol×K	564.66	Joback Method

cpg	268.32	J/mol×K	595.37	Joback Method
dvisc	0.0074186	Pa×s	202.22	Joback Method
dvisc	0.0029798	Pa×s	237.03	Joback Method
dvisc	0.0015119	Pa×s	271.85	Joback Method
dvisc	0.0008949	Pa×s	306.66	Joback Method
dvisc	0.0005894	Pa×s	341.47	Joback Method
dvisc	0.0004194	Pa×s	376.29	Joback Method
dvisc	0.0003162	Pa×s	411.10	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.49996e+01
Coeff. B	-4.00228e+03
Coeff. C	-6.26780e+01
Temperature range (K), min.	334.72
Temperature range (K), max.	475.79

Sources

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

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

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

The Yaws Handbook of Vapor Pressure: https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62017167&Units=SI

Legend

af: Acentric Factor

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume