Hexane, 2,2-dichloro-

Other names: 2,2-dichlorohexane
Inchi: InChI=1S/C6H12Cl2/c1-3-4-5-6(2,7)8/h3-5H2,1-2H3
InchiKey: SJDNOQZXJRUKDE-UHFFFAOYSA-N
Formula: C6H12Cl2
SMILES: CCCCC(C)(Cl)Cl
Mol. weight [g/mol]: 155.06
CAS: 42131-89-5

Physical Properties

Property code	Value	Unit	Source
gf	-21.38	kJ/mol	Joback Method
hf	-207.40	kJ/mol	Joback Method
hfus	12.28	kJ/mol	Joback Method
hvap	36.42	kJ/mol	Joback Method
log10ws	-3.25		Crippen Method
logp	3.370		Crippen Method
mcvol	119.880	ml/mol	McGowan Method
pc	2925.00	kPa	Joback Method
rinpol	925.00		NIST Webbook
rinpol	924.00		NIST Webbook
rinpol	925.00		NIST Webbook
rinpol	925.00		NIST Webbook
ripol	1136.00		NIST Webbook
ripol	1136.00		NIST Webbook
tb	408.31	K	Joback Method
tc	600.47	K	Joback Method
tf	219.64	K	Joback Method
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	214.29	J/mol×K	408.31	Joback Method
cpg	225.73	J/mol×K	440.34	Joback Method

cpg	236.52	J/mol×K	472.36	Joback Method
cpg	246.68	J/mol×K	504.39	Joback Method
cpg	256.26	J/mol×K	536.42	Joback Method
cpg	265.28	J/mol×K	568.45	Joback Method
cpg	273.76	J/mol×K	600.47	Joback Method
dvisc	0.0076476	Pa×s	219.64	Joback Method
dvisc	0.0033292	Pa×s	251.09	Joback Method
dvisc	0.0017440	Pa×s	282.53	Joback Method
dvisc	0.0010399	Pa×s	313.98	Joback Method
dvisc	0.0006813	Pa×s	345.42	Joback Method
dvisc	0.0004790	Pa×s	376.87	Joback Method
dvisc	0.0003555	Pa×s	408.31	Joback Method

Correlations

Information	Value
Property code	pvap
Equation	ln(Pvp) = A + B/(T + C)
Coeff. A	1.52901e+01
Coeff. B	-4.08460e+03
Coeff. C	-6.54580e+01
Temperature range (K), min.	337.72
Temperature range (K), max.	474.79

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C42131895&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

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