Hexane, 3,3-dichloro

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

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	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
rinpol	944.00		NIST Webbook
ripol	1144.00		NIST Webbook
ripol	1144.00		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

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R116082&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
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

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