

2-Hexanone, 1,1-dichloro

Inchi:	InChI=1S/C6H10Cl2O/c1-2-3-4-5(9)6(7)8/h6H,2-4H2,1H3
InchiKey:	AVKICCCNTFCREG-UHFFFAOYSA-N
Formula:	C6H10Cl2O
SMILES:	CCCCC(=O)C(Cl)Cl
Mol. weight [g/mol]:	169.05

Physical Properties

Property code	Value	Unit	Source
gf	-155.58	kJ/mol	Joback Method
hf	-316.51	kJ/mol	Joback Method
hfus	17.77	kJ/mol	Joback Method
hvap	44.08	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.549		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpola	968.00		NIST Webbook
rinpola	968.00		NIST Webbook
tb	464.97	K	Joback Method
tc	660.74	K	Joback Method
tf	252.15	K	Joback Method
vc	0.469	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.76	J/molxK	464.97	Joback Method
cpg	271.63	J/molxK	628.11	Joback Method
cpg	263.76	J/molxK	595.48	Joback Method
cpg	255.45	J/molxK	562.86	Joback Method
cpg	246.69	J/molxK	530.23	Joback Method
cpg	237.47	J/molxK	497.60	Joback Method
cpg	279.08	J/molxK	660.74	Joback Method
dvisc	0.0003532	Paxs	464.97	Joback Method

dvisc	0.0004612	Paxs	429.50	Joback Method
dvisc	0.0006319	Paxs	394.03	Joback Method
dvisc	0.0009213	Paxs	358.56	Joback Method
dvisc	0.0014593	Paxs	323.09	Joback Method
dvisc	0.0025891	Paxs	287.62	Joback Method
dvisc	0.0053974	Paxs	252.15	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R629697&Units=SI

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

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