2-Hexanone, 1,3-dichloro

Inchi: InChI=1S/C6H10Cl2O/c1-2-3-5(8)6(9)4-7/h5H,2-4H2,1H3
InchiKey: CICHFLZUYWZVLC-UHFFFAOYSA-N
Formula: C6H10Cl2O
SMILES: CCCC(Cl)C(=O)CCl
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	-2.03		Crippen Method
logp	2.202		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3096.73	kPa	Joback Method
rinpol	1018.00		NIST Webbook
rinpol	1018.00		NIST Webbook
tb	464.97	K	Joback Method
tc	660.74	K	Joback Method
tf	252.15	K	Joback Method
vc	0.469	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.76	J/mol×K	464.97	Joback Method
cpg	237.47	J/mol×K	497.60	Joback Method
cpg	246.69	J/mol×K	530.23	Joback Method
cpg	255.45	J/mol×K	562.86	Joback Method
cpg	263.76	J/mol×K	595.48	Joback Method
cpg	271.63	J/mol×K	628.11	Joback Method
cpg	279.08	J/mol×K	660.74	Joback Method
dvisc	0.0053974	Pa×s	252.15	Joback Method

dvisc	0.0025891	Pa×s	287.62	Joback Method
dvisc	0.0014593	Pa×s	323.09	Joback Method
dvisc	0.0009213	Pa×s	358.56	Joback Method
dvisc	0.0006319	Pa×s	394.03	Joback Method
dvisc	0.0004612	Pa×s	429.50	Joback Method
dvisc	0.0003532	Pa×s	464.97	Joback Method

Sources

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=R629726&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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