2-Hexanone, 3,3-dichloro

Inchi: InChI=1S/C6H10Cl2O/c1-3-4-6(7,8)5(2)9/h3-4H2,1-2H3
InchiKey: WDQSNLKSSOWOKV-UHFFFAOYSA-N
Formula: C6H10Cl2O
SMILES: CCCC(Cl)(Cl)C(C)=O
Mol. weight [g/mol]: 169.05

Physical Properties

Property code	Value	Unit	Source
gf	-150.30	kJ/mol	Joback Method
hf	-319.98	kJ/mol	Joback Method
hfus	13.88	kJ/mol	Joback Method
hvap	43.17	kJ/mol	Joback Method
log10ws	-2.53		Crippen Method
logp	2.549		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	929.00		NIST Webbook
rinpol	929.00		NIST Webbook
tb	462.18	K	Joback Method
tc	666.21	K	Joback Method
tf	269.57	K	Joback Method
vc	0.465	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.68	J/mol×K	462.18	Joback Method
cpg	276.51	J/mol×K	632.20	Joback Method
cpg	268.54	J/mol×K	598.20	Joback Method
cpg	260.00	J/mol×K	564.19	Joback Method
cpg	250.87	J/mol×K	530.19	Joback Method
cpg	241.10	J/mol×K	496.18	Joback Method
cpg	283.96	J/mol×K	666.21	Joback Method
dvisc	0.0003744	Pa×s	462.18	Joback Method

dvisc	0.0004930	Pa×s	430.08	Joback Method
dvisc	0.0006788	Pa×s	397.98	Joback Method
dvisc	0.0009885	Pa×s	365.88	Joback Method
dvisc	0.0015473	Pa×s	333.77	Joback Method
dvisc	0.0026645	Pa×s	301.67	Joback Method
dvisc	0.0052226	Pa×s	269.57	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629766&Units=SI
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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