2-Hexanone, 3-chloro

Inchi: InChI=1S/C6H11ClO/c1-3-4-6(7)5(2)8/h6H,3-4H2,1-2H3
InchiKey: BMAOXIKHKBCNHU-UHFFFAOYSA-N
Formula: C6H11ClO
SMILES: CCCC(Cl)C(C)=O
Mol. weight [g/mol]: 134.60

Physical Properties

Property code	Value	Unit	Source
gf	-143.65	kJ/mol	Joback Method
hf	-300.77	kJ/mol	Joback Method
hfus	13.57	kJ/mol	Joback Method
hvap	39.69	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.983		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	884.00		NIST Webbook
rinpol	884.00		NIST Webbook
tb	427.54	K	Joback Method
tc	616.78	K	Joback Method
tf	222.23	K	Joback Method
vc	0.420	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.25	J/mol×K	427.54	Joback Method
cpg	249.52	J/mol×K	585.24	Joback Method
cpg	241.12	J/mol×K	553.70	Joback Method
cpg	232.30	J/mol×K	522.16	Joback Method
cpg	223.06	J/mol×K	490.62	Joback Method
cpg	213.38	J/mol×K	459.08	Joback Method
cpg	257.52	J/mol×K	616.78	Joback Method
dvisc	0.0003354	Pa×s	427.54	Joback Method

dvisc	0.0004397	Pa×s	393.32	Joback Method
dvisc	0.0006070	Pa×s	359.10	Joback Method
dvisc	0.0008968	Pa×s	324.88	Joback Method
dvisc	0.0014525	Pa×s	290.67	Joback Method
dvisc	0.0026756	Pa×s	256.45	Joback Method
dvisc	0.0059488	Pa×s	222.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629786&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