

3-Hexanone, 4-chloro

Inchi:	InChI=1S/C6H11ClO/c1-3-5(7)6(8)4-2/h5H,3-4H2,1-2H3
InchiKey:	JLRAWVOPMUYZEP-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	CCC(=O)C(Cl)CC
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
mvol	109.210	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	888.00		NIST Webbook
rinpol	888.00		NIST Webbook
tb	427.54	K	Joback Method
tc	616.78	K	Joback Method
tf	222.23	K	Joback Method
vc	0.420	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.25	J/molxK	427.54	Joback Method
cpg	213.38	J/molxK	459.08	Joback Method
cpg	223.06	J/molxK	490.62	Joback Method
cpg	232.30	J/molxK	522.16	Joback Method
cpg	241.12	J/molxK	553.70	Joback Method
cpg	249.52	J/molxK	585.24	Joback Method
cpg	257.52	J/molxK	616.78	Joback Method
dvisc	0.0059488	Paxs	222.23	Joback Method

dvisc	0.0026756	Paxs	256.45	Joback Method
dvisc	0.0014525	Paxs	290.67	Joback Method
dvisc	0.0008968	Paxs	324.88	Joback Method
dvisc	0.0006070	Paxs	359.10	Joback Method
dvisc	0.0004397	Paxs	393.32	Joback Method
dvisc	0.0003354	Paxs	427.54	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=R630236&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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