

2-Hexanone, 3-chloro-4-methyl

Inchi:	InChI=1S/C7H13ClO/c1-4-5(2)7(8)6(3)9/h5,7H,4H2,1-3H3
InchiKey:	DVQTVIPKAAGOPF-UHFFFAOYSA-N
Formula:	C7H13ClO
SMILES:	CCC(C)C(Cl)C(C)=O
Mol. weight [g/mol]:	148.63

Physical Properties

Property code	Value	Unit	Source
gf	-137.67	kJ/mol	Joback Method
hf	-326.69	kJ/mol	Joback Method
hfus	12.64	kJ/mol	Joback Method
hvap	41.53	kJ/mol	Joback Method
log10ws	-2.06		Crippen Method
logp	2.229		Crippen Method
mcvol	123.300	ml/mol	McGowan Method
pc	2928.17	kPa	Joback Method
rinpol	940.00		NIST Webbook
rinpol	940.00		NIST Webbook
tb	449.98	K	Joback Method
tc	641.72	K	Joback Method
tf	218.50	K	Joback Method
vc	0.470	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	242.70	J/molxK	449.98	Joback Method
cpg	254.38	J/molxK	481.94	Joback Method
cpg	265.53	J/molxK	513.89	Joback Method
cpg	276.15	J/molxK	545.85	Joback Method
cpg	286.27	J/molxK	577.81	Joback Method
cpg	295.89	J/molxK	609.77	Joback Method
cpg	305.03	J/molxK	641.72	Joback Method
dvisc	0.0095406	Paxs	218.50	Joback Method

dvisc	0.0034936	Paxs	257.08	Joback Method
dvisc	0.0016628	Paxs	295.66	Joback Method
dvisc	0.0009394	Paxs	334.24	Joback Method
dvisc	0.0005973	Paxs	372.82	Joback Method
dvisc	0.0004134	Paxs	411.40	Joback Method
dvisc	0.0003048	Paxs	449.98	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R629791&Units=SI
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

Legend

cp_g:	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:	Log ₁₀ of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
m_{cvol}:	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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