

2-Pentanone, 3-chloro-4-methyl

Inchi:	InChI=1S/C6H11ClO/c1-4(2)6(7)5(3)8/h4,6H,1-3H3
InchiKey:	OLBUMMGFVTVKFF-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	CC(=O)C(Cl)C(C)C
Mol. weight [g/mol]:	134.60

Physical Properties

Property code	Value	Unit	Source
gf	-146.09	kJ/mol	Joback Method
hf	-306.05	kJ/mol	Joback Method
hfus	10.05	kJ/mol	Joback Method
hvap	39.31	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.839		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3257.86	kPa	Joback Method
rinpola	850.00		NIST Webbook
rinpola	850.00		NIST Webbook
tb	427.10	K	Joback Method
tc	620.79	K	Joback Method
tf	207.23	K	Joback Method
vc	0.414	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	203.33	J/molxK	427.10	Joback Method
cpg	250.96	J/molxK	588.51	Joback Method
cpg	242.34	J/molxK	556.23	Joback Method
cpg	233.28	J/molxK	523.94	Joback Method
cpg	223.77	J/molxK	491.66	Joback Method
cpg	213.79	J/molxK	459.38	Joback Method
cpg	259.15	J/molxK	620.79	Joback Method
dvisc	0.0003215	Paxs	427.10	Joback Method

dvisc	0.0004344	Paxs	390.46	Joback Method
dvisc	0.0006245	Paxs	353.81	Joback Method
dvisc	0.0009763	Paxs	317.17	Joback Method
dvisc	0.0017155	Paxs	280.52	Joback Method
dvisc	0.0035708	Paxs	243.88	Joback Method
dvisc	0.0096323	Paxs	207.23	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R630003&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
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

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