

2-Pentanone, 1-chloro-4-methyl

Inchi:	InChI=1S/C6H11ClO/c1-5(2)3-6(8)4-7/h5H,3-4H2,1-2H3
InchiKey:	QVMRSFQXWJGXRL-UHFFFAOYSA-N
Formula:	C6H11ClO
SMILES:	CC(C)CC(=O)CCl
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	-1.53		Crippen Method
logp	1.840		Crippen Method
mvol	109.210	ml/mol	McGowan Method
pc	3228.31	kPa	Joback Method
rinpol	942.00		NIST Webbook
rinpol	942.00		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/mol×K	427.54	Joback Method
cpg	213.38	J/mol×K	459.08	Joback Method
cpg	223.06	J/mol×K	490.62	Joback Method
cpg	232.30	J/mol×K	522.16	Joback Method
cpg	241.12	J/mol×K	553.70	Joback Method
cpg	249.52	J/mol×K	585.24	Joback Method
cpg	257.52	J/mol×K	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

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=R629984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
h_{vap}:	Enthalpy of vaporization at standard conditions
log₁₀ws:	Log ₁₀ of Water solubility in mol/l
log_p:	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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