2-Butanone, 1-chloro-3-methyl

Inchi: InChI=1S/C5H9ClO/c1-4(2)5(7)3-6/h4H,3H2,1-2H3
InchiKey: GGTWUPLPAPTFAR-UHFFFAOYSA-N
Formula: C5H9ClO
SMILES: CC(C)C(=O)CCl
Mol. weight [g/mol]: 120.58

Physical Properties

Property code	Value	Unit	Source
gf	-152.07	kJ/mol	Joback Method
hf	-280.13	kJ/mol	Joback Method
hfus	10.98	kJ/mol	Joback Method
hvap	37.47	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.450		Crippen Method
mcvol	95.120	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
rinpol	820.00		NIST Webbook
tb	404.66	K	Joback Method
tc	595.49	K	Joback Method
tf	210.96	K	Joback Method
vc	0.364	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	166.21	J/mol×K	404.66	Joback Method
cpg	174.99	J/mol×K	436.47	Joback Method
cpg	183.38	J/mol×K	468.27	Joback Method
cpg	191.40	J/mol×K	500.08	Joback Method
cpg	199.04	J/mol×K	531.88	Joback Method
cpg	206.34	J/mol×K	563.69	Joback Method
cpg	213.28	J/mol×K	595.49	Joback Method
dvisc	0.0057299	Pa×s	210.96	Joback Method
dvisc	0.0026320	Pa×s	243.24	Joback Method

dvisc	0.0014508	Pa×s	275.53	Joback Method
dvisc	0.0009061	Pa×s	307.81	Joback Method
dvisc	0.0006188	Pa×s	340.09	Joback Method
dvisc	0.0004515	Pa×s	372.38	Joback Method
dvisc	0.0003464	Pa×s	404.66	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=R629528&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