2-Butanone, 1,1-dichloro-3,3-dimethyl-

Other names:	1,1-Dichloro-3,3-dimethyl-2-butanone
	Dichloromethyl tert-butyl ketone
	Dichloropinacolin
	«alpha»,«alpha»-Dichloropinacolin
	Dichloropinakolin
	«omega»,«omega»-Dichlorpinakolin
	1,1-dichloro-3,3-dimethylbutan-2-one
Inchi:	InChI=1S/C6H10Cl2O/c1-6(2,3)4(9)5(7)8/h5H,1-3H3
InchiKey:	UDWZXMQIEHAAQT-UHFFFAOYSA-N
Formula:	C6H10Cl2O
SMILES:	CC(C)(C)C(=O)C(Cl)Cl
Mol. weight [g/mol]:	169.05
CAS:	22591-21-5

Physical Properties

Property code	Value	Unit	Source
gf	-152.74	kJ/mol	Joback Method
hf	-325.26	kJ/mol	Joback Method
hfus	10.35	kJ/mol	Joback Method
hvap	42.78	kJ/mol	Joback Method
log10ws	-2.29		Crippen Method
logp	2.405		Crippen Method
mcvol	121.450	ml/mol	McGowan Method
pc	3163.27	kPa	Joback Method
tb	461.74	K	Joback Method
tc	670.58	K	Joback Method
tf	321.20 ± 0.50	K	NIST Webbook
tf	324.00 ± 2.00	K	NIST Webbook
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	230.86	J/mol×K	461.74	Joback Method

cpg	241.62	J/mol×K	496.55	Joback Method
cpg	251.67	J/mol×K	531.35	Joback Method
cpg	261.06	J/mol×K	566.16	Joback Method
cpg	269.82	J/mol×K	600.97	Joback Method
cpg	277.98	J/mol×K	635.77	Joback Method
cpg	285.58	J/mol×K	670.58	Joback Method
dvisc	0.0076920	Pa×s	254.57	Joback Method
dvisc	0.0033961	Pa×s	289.10	Joback Method
dvisc	0.0017852	Pa×s	323.63	Joback Method
dvisc	0.0010623	Pa×s	358.15	Joback Method
dvisc	0.0006925	Pa×s	392.68	Joback Method
dvisc	0.0004838	Pa×s	427.21	Joback Method
dvisc	0.0003566	Pa×s	461.74	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C22591215&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Joback Method:	https://en.wikipedia.org/wiki/Joback_method

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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume