2-Butanone, 1-chloro-3,3-dimethyl-

Other names: 1-Chloro-3,3-dimethyl-2-butanone
«alpha»-Chloropinacolone
Chloromethyl tert-butyl ketone
tert-Butyl chloromethyl ketone
1-Chloropinacolone
1-chloro-3,3-dimethylbutan-2-one
Inchi: InChI=1S/C6H11ClO/c1-6(2,3)5(8)4-7/h4H2,1-3H3
InchiKey: ULSAJQMHTGKPIY-UHFFFAOYSA-N
Formula: C6H11ClO
SMILES: CC(C)(C)C(=O)CCl
Mol. weight [g/mol]: 134.60
CAS: 13547-70-1

Physical Properties

Property code	Value	Unit	Source
gf	-138.37	kJ/mol	Joback Method
hf	-304.24	kJ/mol	Joback Method
hfus	9.68	kJ/mol	Joback Method
hvap	38.78	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.840		Crippen Method
mcvol	109.210	ml/mol	McGowan Method
pc	3269.04	kPa	Joback Method
rinpol	915.00		NIST Webbook
rinpol	915.00		NIST Webbook
tb	444.70	K	NIST Webbook
tc	622.09	K	Joback Method
tf	260.55 ± 0.50	K	NIST Webbook
vc	0.415	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	205.61	J/mol×K	424.75	Joback Method

cpg	254.69	J/mol×K	589.20	Joback Method
cpg	246.04	J/mol×K	556.31	Joback Method
cpg	236.83	J/mol×K	523.42	Joback Method
cpg	227.04	J/mol×K	490.53	Joback Method
cpg	216.65	J/mol×K	457.64	Joback Method
cpg	262.82	J/mol×K	622.09	Joback Method
dvisc	0.0003699	Pa×s	424.75	Joback Method
dvisc	0.0004907	Pa×s	393.90	Joback Method
dvisc	0.0006831	Pa×s	363.05	Joback Method
dvisc	0.0010112	Pa×s	332.20	Joback Method
dvisc	0.0016221	Pa×s	301.35	Joback Method
dvisc	0.0028981	Pa×s	270.50	Joback Method
dvisc	0.0060123	Pa×s	239.65	Joback Method

Sources

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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13547701&Units=SI

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