Propanoic acid, 3-chloro-2,2-dimethyl-

Other names:	Propionic acid, 3-chloro-2,2-dimethyl- «beta»-Chloro-«alpha»,«alpha»-dimethylpropionic acid «beta»-Chloropivalic acid Chloropivalic acid Chlorotrimethylacetic acid 3-Chloro-2,2-dimethylpropionic acid 3-Chloropivalic acid NSC 89696 3-chloro-2,2-dimethylpropaneoic acid
Inchi:	InChI=1S/C5H9ClO2/c1-5(2,3-6)4(7)8/h3H2,1-2H3,(H,7,8)
InchiKey:	YBJGQSNSAWZZHL-UHFFFAOYSA-N
Formula:	C5H9ClO2
SMILES:	CC(C)(CCl)C(=O)O
Mol. weight [g/mol]:	136.58
CAS:	13511-38-1

Physical Properties

Property code	Value	Unit	Source
gf	-283.61	kJ/mol	Joback Method
hf	-435.83	kJ/mol	Joback Method
hfus	11.18	kJ/mol	Joback Method
hvap	53.24	kJ/mol	Joback Method
log10ws	-0.93		Crippen Method
logp	1.336		Crippen Method
mcvol	100.990	ml/mol	McGowan Method
pc	4103.88	kPa	Joback Method
tb	488.20	K	NIST Webbook
tc	683.23	K	Joback Method
tf	314.00 ± 4.00	K	NIST Webbook
vc	0.379	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	209.78	J/mol×K	494.05	Joback Method
cpg	217.91	J/mol×K	525.58	Joback Method
cpg	225.55	J/mol×K	557.11	Joback Method
cpg	232.72	J/mol×K	588.64	Joback Method
cpg	239.44	J/mol×K	620.17	Joback Method
cpg	245.76	J/mol×K	651.70	Joback Method
cpg	251.67	J/mol×K	683.23	Joback Method
dvisc	0.0199748	Pa×s	289.20	Joback Method
dvisc	0.0063037	Pa×s	323.34	Joback Method
dvisc	0.0024796	Pa×s	357.48	Joback Method
dvisc	0.0011477	Pa×s	391.62	Joback Method
dvisc	0.0006011	Pa×s	425.77	Joback Method
dvisc	0.0003465	Pa×s	459.91	Joback Method
dvisc	0.0002156	Pa×s	494.05	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	383.20	K	1.30	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C13511381&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
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
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume