

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

Other names:	Propionic acid, 3-chloro-2,2-dimethyl-, methyl ester Methyl chloropivalate
Inchi:	InChI=1S/C6H11ClO2/c1-6(2,4-7)5(8)9-3/h4H2,1-3H3
InchiKey:	CKYBSQGDQJXNSB-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	COC(=O)C(C)(C)CCl
Mol. weight [g/mol]:	150.60
CAS:	21491-96-3

Physical Properties

Property code	Value	Unit	Source
gf	-243.37	kJ/mol	Joback Method
hf	-436.46	kJ/mol	Joback Method
hfus	10.87	kJ/mol	Joback Method
hvap	41.20	kJ/mol	Joback Method
log10ws	-1.11		Crippen Method
logp	1.424		Crippen Method
mvol	115.080	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
tb	447.17	K	Joback Method
tc	643.60	K	Joback Method
tf	261.88	K	Joback Method
vc	0.433	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	227.74	J/molxK	447.17	Joback Method
cpg	275.92	J/molxK	610.86	Joback Method
cpg	267.31	J/molxK	578.12	Joback Method
cpg	258.20	J/molxK	545.38	Joback Method
cpg	248.58	J/molxK	512.65	Joback Method
cpg	238.43	J/molxK	479.91	Joback Method
cpg	284.06	J/molxK	643.60	Joback Method

dvisc	0.0003084	Paxs	447.17	Joback Method
dvisc	0.0004059	Paxs	416.29	Joback Method
dvisc	0.0005582	Paxs	385.41	Joback Method
dvisc	0.0008115	Paxs	354.52	Joback Method
dvisc	0.0012671	Paxs	323.64	Joback Method
dvisc	0.0021735	Paxs	292.76	Joback Method
dvisc	0.0042341	Paxs	261.88	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C21491963&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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