Propanoic acid, 2,2-dimethyl-, chloromethyl ester

Other names:	Chloromethyl pivalate
	Pivalic acid chloromethyl ester
Inchi:	InChI=1S/C6H11ClO2/c1-6(2,3)5(8)9-4-7/h4H2,1-3H3
InchiKey:	GGRHYQCXXYLUTL-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CC(C)(C)C(=O)OCCl
Mol. weight [g/mol]:	150.60
CAS:	18997-19-8

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	-1.60		Crippen Method
logp	1.772		Crippen Method
mcvol	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	m3/kmol	Joback Method

Temperature Dependent Properties

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

dvisc	0.0042341	Pa×s	261.88	Joback Method
dvisc	0.0021735	Pa×s	292.76	Joback Method
dvisc	0.0012671	Pa×s	323.64	Joback Method
dvisc	0.0008115	Pa×s	354.52	Joback Method
dvisc	0.0005582	Pa×s	385.41	Joback Method
dvisc	0.0004059	Pa×s	416.29	Joback Method
dvisc	0.0003084	Pa×s	447.17	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=C18997198&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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