Acetic acid, chloro-, 1,1-dimethylethyl ester

Other names:	Acetic acid, chloro-, tert-butyl ester
	tert-Butyl Chloroacetate
	Chloroacetic acid tert-butyl ester
	ClCH2C(O)OC(CH3)3
Inchi:	InChI=1S/C6H11ClO2/c1-6(2,3)9-5(8)4-7/h4H2,1-3H3
InchiKey:	KUYMVWXKHQSIAS-UHFFFAOYSA-N
Formula:	C6H11ClO2
SMILES:	CC(C)(C)OC(=O)CCl
Mol. weight [g/mol]:	150.60
CAS:	107-59-5

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	-1.46		Crippen Method
logp	1.567		Crippen Method
mcvol	115.080	ml/mol	McGowan Method
pc	3206.41	kPa	Joback Method
rinpol	891.00		NIST Webbook
ripol	1280.00		NIST Webbook
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

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	321.70	K	1.50	NIST Webbook

Sources

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=C107595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
ripol:	Polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume