Chloroacetic acid, 3-methylbut-2-yl ester

Other names: Acetic acid, chloro, 1,2-dimethylpropyl ester
Inchi: InChI=1S/C7H13ClO2/c1-5(2)6(3)10-7(9)4-8/h5-6H,4H2,1-3H3
InchiKey: YOUOQIIPGBGSJE-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CC(C)C(C)OC(=O)CCl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-242.67	kJ/mol	Joback Method
hf	-458.91	kJ/mol	Joback Method
hfus	13.82	kJ/mol	Joback Method
hvap	43.94	kJ/mol	Joback Method
log10ws	-1.64		Crippen Method
logp	1.813		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
rinpol	1012.00		NIST Webbook
rinpol	1059.00		NIST Webbook
rinpol	1059.00		NIST Webbook
ripol	1414.00		NIST Webbook
tb	472.40	K	Joback Method
tc	663.16	K	Joback Method
tf	240.73	K	Joback Method
vc	0.488	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	265.59	J/mol×K	472.40	Joback Method
cpg	277.03	J/mol×K	504.19	Joback Method
cpg	288.00	J/mol×K	535.99	Joback Method
cpg	298.52	J/mol×K	567.78	Joback Method
cpg	308.57	J/mol×K	599.57	Joback Method

cpg	318.17	J/mol×K	631.37	Joback Method
cpg	327.32	J/mol×K	663.16	Joback Method
dvisc	0.0064287	Pa×s	240.73	Joback Method
dvisc	0.0025878	Pa×s	279.34	Joback Method
dvisc	0.0012993	Pa×s	317.95	Joback Method
dvisc	0.0007574	Pa×s	356.56	Joback Method
dvisc	0.0004906	Pa×s	395.18	Joback Method
dvisc	0.0003433	Pa×s	433.79	Joback Method
dvisc	0.0002547	Pa×s	472.40	Joback Method

Sources

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=U354603&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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