Acetic acid, chloro, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C7H13ClO2/c1-4-7(2,3)10-6(9)5-8/h4-5H2,1-3H3
InchiKey: KPFTZXFNGNJOQM-UHFFFAOYSA-N
Formula: C7H13ClO2
SMILES: CCC(C)(C)OC(=O)CCl
Mol. weight [g/mol]: 164.63

Physical Properties

Property code	Value	Unit	Source
gf	-234.95	kJ/mol	Joback Method
hf	-457.10	kJ/mol	Joback Method
hfus	13.46	kJ/mol	Joback Method
hvap	43.42	kJ/mol	Joback Method
log10ws	-1.88		Crippen Method
logp	1.957		Crippen Method
mcvol	129.170	ml/mol	McGowan Method
pc	2884.30	kPa	Joback Method
rinpol	995.00		NIST Webbook
rinpol	995.00		NIST Webbook
ripol	1382.00		NIST Webbook
tb	470.05	K	Joback Method
tc	664.25	K	Joback Method
tf	273.15	K	Joback Method
vc	0.489	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	268.23	J/mol×K	470.05	Joback Method
cpg	321.60	J/mol×K	631.88	Joback Method
cpg	312.05	J/mol×K	599.52	Joback Method
cpg	301.96	J/mol×K	567.15	Joback Method
cpg	291.30	J/mol×K	534.78	Joback Method
cpg	280.06	J/mol×K	502.42	Joback Method
cpg	330.63	J/mol×K	664.25	Joback Method

dvisc	0.0002819	Pa×s	470.05	Joback Method
dvisc	0.0003728	Pa×s	437.23	Joback Method
dvisc	0.0005158	Pa×s	404.42	Joback Method
dvisc	0.0007558	Pa×s	371.60	Joback Method
dvisc	0.0011926	Pa×s	338.78	Joback Method
dvisc	0.0020752	Pa×s	305.97	Joback Method
dvisc	0.0041252	Pa×s	273.15	Joback Method

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=R115618&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
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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