Acetic acid, trichloro, 1,1-dimethylpropyl ester

Inchi: InChI=1S/C7H11Cl3O2/c1-4-6(2,3)12-5(11)7(8,9)10/h4H2,1-3H3
InchiKey: IOFGLFCKRVLSBV-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CCC(C)(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 233.52

Physical Properties

Property code	Value	Unit	Source
gf	-255.97	kJ/mol	Joback Method
hf	-497.33	kJ/mol	Joback Method
hfus	14.44	kJ/mol	Joback Method
hvap	50.89	kJ/mol	Joback Method
log10ws	-3.29		Crippen Method
logp	3.088		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2721.17	kPa	Joback Method
rinpol	1147.00		NIST Webbook
rinpol	1147.00		NIST Webbook
ripol	1417.00		NIST Webbook
ripol	1417.00		NIST Webbook
tb	541.68	K	Joback Method
tc	759.32	K	Joback Method
tf	335.41	K	Joback Method
vc	0.577	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	322.35	J/mol×K	541.68	Joback Method
cpg	333.60	J/mol×K	577.95	Joback Method
cpg	344.01	J/mol×K	614.23	Joback Method
cpg	353.63	J/mol×K	650.50	Joback Method
cpg	362.50	J/mol×K	686.77	Joback Method
cpg	370.68	J/mol×K	723.04	Joback Method

cpg	378.22	J/mol×K	759.32	Joback Method
dvisc	0.0033014	Pa×s	335.41	Joback Method
dvisc	0.0017293	Pa×s	369.79	Joback Method
dvisc	0.0010112	Pa×s	404.17	Joback Method
dvisc	0.0006431	Pa×s	438.55	Joback Method
dvisc	0.0004369	Pa×s	472.92	Joback Method
dvisc	0.0003127	Pa×s	507.30	Joback Method
dvisc	0.0002336	Pa×s	541.68	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=R115841&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
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