Acetic acid, trichloro, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C7H11Cl3O2/c1-4(2)5(3)12-6(11)7(8,9)10/h4-5H,1-3H3
InchiKey: DLGMINPBZKHLST-UHFFFAOYSA-N
Formula: C7H11Cl3O2
SMILES: CC(C)C(C)OC(=O)C(Cl)(Cl)Cl
Mol. weight [g/mol]: 233.52

Physical Properties

Property code	Value	Unit	Source
gf	-263.69	kJ/mol	Joback Method
hf	-499.14	kJ/mol	Joback Method
hfus	14.80	kJ/mol	Joback Method
hvap	51.41	kJ/mol	Joback Method
log10ws	-3.05		Crippen Method
logp	2.944		Crippen Method
mcvol	153.650	ml/mol	McGowan Method
pc	2712.67	kPa	Joback Method
rinpol	1163.00		NIST Webbook
rinpol	1163.00		NIST Webbook
ripol	1446.00		NIST Webbook
ripol	1446.00		NIST Webbook
tb	544.03	K	Joback Method
tc	757.75	K	Joback Method
tf	302.99	K	Joback Method
vc	0.576	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	319.41	J/mol×K	544.03	Joback Method
cpg	368.07	J/mol×K	722.13	Joback Method
cpg	359.65	J/mol×K	686.51	Joback Method
cpg	350.61	J/mol×K	650.89	Joback Method
cpg	340.90	J/mol×K	615.27	Joback Method
cpg	330.51	J/mol×K	579.65	Joback Method

cpg	375.88	J/mol×K	757.75	Joback Method
dvisc	0.0002209	Pa×s	544.03	Joback Method
dvisc	0.0003036	Pa×s	503.86	Joback Method
dvisc	0.0004407	Pa×s	463.68	Joback Method
dvisc	0.0006867	Pa×s	423.51	Joback Method
dvisc	0.0011742	Pa×s	383.34	Joback Method
dvisc	0.0022766	Pa×s	343.16	Joback Method
dvisc	0.0052610	Pa×s	302.99	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R115856&Units=SI
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

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