Acetic acid, dichloro, 1,2-dimethylpropyl ester

Inchi: InChI=1S/C7H12Cl2O2/c1-4(2)5(3)11-7(10)6(8)9/h4-6H,1-3H3
InchiKey: VVJYTELLIBXTPJ-UHFFFAOYSA-N
Formula: C7H12Cl2O2
SMILES: CC(C)C(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 199.07

Physical Properties

Property code	Value	Unit	Source
gf	-257.04	kJ/mol	Joback Method
hf	-479.93	kJ/mol	Joback Method
hfus	14.50	kJ/mol	Joback Method
hvap	47.94	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.378		Crippen Method
mcvol	141.410	ml/mol	McGowan Method
pc	2787.66	kPa	Joback Method
rinpol	1084.00		NIST Webbook
rinpol	1084.00		NIST Webbook
ripol	1476.00		NIST Webbook
ripol	1476.00		NIST Webbook
tb	509.39	K	Joback Method
tc	710.00	K	Joback Method
tf	255.65	K	Joback Method
vc	0.531	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	291.53	J/mol×K	509.39	Joback Method
cpg	342.67	J/mol×K	676.56	Joback Method
cpg	333.48	J/mol×K	643.13	Joback Method
cpg	323.78	J/mol×K	609.69	Joback Method
cpg	313.56	J/mol×K	576.26	Joback Method
cpg	302.81	J/mol×K	542.82	Joback Method

cpg	351.35	J/mol×K	710.00	Joback Method
dvisc	0.0002372	Pa×s	509.39	Joback Method
dvisc	0.0003263	Pa×s	467.10	Joback Method
dvisc	0.0004782	Pa×s	424.81	Joback Method
dvisc	0.0007628	Pa×s	382.52	Joback Method
dvisc	0.0013664	Pa×s	340.23	Joback Method
dvisc	0.0028881	Pa×s	297.94	Joback Method
dvisc	0.0078195	Pa×s	255.65	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R115727&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

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