Acetic acid, dichloro-, 1,1-dimethylethyl ester

Other names: 1,1-dimethylethyl dichloroacetate
Inchi: InChI=1S/C6H10Cl2O2/c1-6(2,3)10-5(9)4(7)8/h4H,1-3H3
InchiKey: FOLRKRMAFDGZRR-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: CC(C)(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 185.05
CAS: 49653-47-6

Physical Properties

Property code	Value	Unit	Source
gf	-257.74	kJ/mol	Joback Method
hf	-457.48	kJ/mol	Joback Method
hfus	11.54	kJ/mol	Joback Method
hvap	45.19	kJ/mol	Joback Method
log10ws	-2.22		Crippen Method
logp	2.132		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3103.64	kPa	Joback Method
rinpol	960.00		NIST Webbook
rinpol	960.00		NIST Webbook
ripol	1339.00		NIST Webbook
ripol	1339.00		NIST Webbook
tb	484.16	K	Joback Method
tc	691.34	K	Joback Method
tf	276.80	K	Joback Method
vc	0.476	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	252.57	J/mol×K	484.16	Joback Method
cpg	263.03	J/mol×K	518.69	Joback Method
cpg	272.88	J/mol×K	553.22	Joback Method
cpg	282.14	J/mol×K	587.75	Joback Method

cpg	290.84	J/mol×K	622.28	Joback Method
cpg	298.99	J/mol×K	656.81	Joback Method
cpg	306.61	J/mol×K	691.34	Joback Method
dvisc	0.0051343	Pa×s	276.80	Joback Method
dvisc	0.0024308	Pa×s	311.36	Joback Method
dvisc	0.0013363	Pa×s	345.92	Joback Method
dvisc	0.0008189	Pa×s	380.48	Joback Method
dvisc	0.0005445	Pa×s	415.04	Joback Method
dvisc	0.0003855	Pa×s	449.60	Joback Method
dvisc	0.0002867	Pa×s	484.16	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C49653476&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