Acetic acid, dichloro-, 1-methylethyl ester

Other names: Isopropyl dichloroacetate
Inchi: InChI=1S/C5H8Cl2O2/c1-3(2)9-5(8)4(6)7/h3-4H,1-2H3
InchiKey: JBTISLVNJCYZCH-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: CC(C)OC(=O)C(Cl)Cl
Mol. weight [g/mol]: 171.02
CAS: 25006-60-4

Physical Properties

Property code	Value	Unit	Source
chl	-2618.00 ± 4.00	kJ/mol	NIST Webbook
chl	-2613.00	kJ/mol	NIST Webbook
gf	-271.44	kJ/mol	Joback Method
hf	-433.37	kJ/mol	Joback Method
hfus	12.84	kJ/mol	Joback Method
hvap	43.87	kJ/mol	Joback Method
log10ws	-1.80		Crippen Method
logp	1.742		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3419.86	kPa	Joback Method
rinpol	918.00		NIST Webbook
rinpol	918.00		NIST Webbook
rinpol	920.80		NIST Webbook
ripol	1345.00		NIST Webbook
ripol	1345.00		NIST Webbook
tb	464.07	K	Joback Method
tc	665.53	K	Joback Method
tf	248.11	K	Joback Method
vc	0.425	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.76	J/mol×K	464.07	Joback Method

cpg	248.84	J/mol×K	631.95	Joback Method
cpg	241.76	J/mol×K	598.37	Joback Method
cpg	234.31	J/mol×K	564.80	Joback Method
cpg	226.49	J/mol×K	531.22	Joback Method
cpg	218.31	J/mol×K	497.65	Joback Method
cpg	255.55	J/mol×K	665.53	Joback Method
dvisc	0.0003006	Pa×s	464.07	Joback Method
dvisc	0.0003993	Pa×s	428.08	Joback Method
dvisc	0.0005589	Pa×s	392.08	Joback Method
dvisc	0.0008373	Pa×s	356.09	Joback Method
dvisc	0.0013736	Pa×s	320.10	Joback Method
dvisc	0.0025548	Pa×s	284.10	Joback Method
dvisc	0.0056889	Pa×s	248.11	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C25006604&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

chl: Standard liquid enthalpy of combustion
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