Dichloroacetic acid 2-methylpropyl ester

Other names: Acetic acid, dichloro, 2-methylpropyl ester
Acetic acid, dichloro, isobutyl ester
Isobutyl dichloroacetate
Inchi: InChI=1S/C6H10Cl2O2/c1-4(2)3-10-6(9)5(7)8/h4-5H,3H2,1-2H3
InchiKey: XLKJPQKUATYFQJ-UHFFFAOYSA-N
Formula: C6H10Cl2O2
SMILES: CC(C)COC(=O)C(Cl)Cl
Mol. weight [g/mol]: 185.05
CAS: 37079-08-6

Physical Properties

Property code	Value	Unit	Source
chl	-3274.00	kJ/mol	NIST Webbook
chl	-3278.70 ± 4.20	kJ/mol	NIST Webbook
gf	-263.02	kJ/mol	Joback Method
hf	-501.70 ± 9.60	kJ/mol	NIST Webbook
hfl	-554.00 ± 8.40	kJ/mol	NIST Webbook
hfus	15.43	kJ/mol	Joback Method
hvap	52.30 ± 4.20	kJ/mol	NIST Webbook
log10ws	-1.87		Crippen Method
logp	1.989		Crippen Method
mcvol	127.320	ml/mol	McGowan Method
pc	3065.95	kPa	Joback Method
rinpol	1030.00		NIST Webbook
rinpol	1030.00		NIST Webbook
rinpol	1028.80		NIST Webbook
ripol	1458.00		NIST Webbook
ripol	1458.00		NIST Webbook
tb	486.95	K	Joback Method
tc	685.84	K	Joback Method
tf	259.38	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	301.92	J/mol×K	685.84	Joback Method
cpg	249.45	J/mol×K	486.95	Joback Method
cpg	259.28	J/mol×K	520.10	Joback Method
cpg	268.68	J/mol×K	553.25	Joback Method
cpg	277.63	J/mol×K	586.39	Joback Method
cpg	286.16	J/mol×K	619.54	Joback Method
cpg	294.25	J/mol×K	652.69	Joback Method
dvisc	0.0002759	Pa×s	486.95	Joback Method
dvisc	0.0055114	Pa×s	259.38	Joback Method
dvisc	0.0024337	Pa×s	297.31	Joback Method
dvisc	0.0012930	Pa×s	335.24	Joback Method
dvisc	0.0007812	Pa×s	373.16	Joback Method
dvisc	0.0005180	Pa×s	411.09	Joback Method
dvisc	0.0003681	Pa×s	449.02	Joback Method
hvapt	51.40	kJ/mol	378.50	NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37079086&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

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
hfl: Liquid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions

hvap:	Enthalpy of vaporization at standard conditions
hvapt:	Enthalpy of vaporization at a given temperature
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