2,2-dichloroethyl propionate

Inchi: InChI=1S/C5H8Cl2O2/c1-2-5(8)9-3-4(6)7/h4H,2-3H2,1H3
InchiKey: WYEIXHWXQYAHAM-UHFFFAOYSA-N
Formula: C5H8Cl2O2
SMILES: CCC(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 171.02

Physical Properties

Property code	Value	Unit	Source
gf	-269.00	kJ/mol	Joback Method
hf	-428.09	kJ/mol	Joback Method
hfus	16.36	kJ/mol	Joback Method
hvap	44.26	kJ/mol	Joback Method
log10ws	-1.69		Crippen Method
logp	1.743		Crippen Method
mcvol	113.230	ml/mol	McGowan Method
pc	3388.08	kPa	Joback Method
rinpol	997.00		NIST Webbook
rinpol	1010.00		NIST Webbook
rinpol	991.00		NIST Webbook
rinpol	989.00		NIST Webbook
rinpol	988.00		NIST Webbook
rinpol	997.00		NIST Webbook
ripol	1495.00		NIST Webbook
ripol	1545.00		NIST Webbook
ripol	1527.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1513.00		NIST Webbook
tb	464.51	K	Joback Method
tc	661.42	K	Joback Method
tf	263.11	K	Joback Method
vc	0.431	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	209.55	J/mol×K	464.51	Joback Method
cpg	247.49	J/mol×K	628.60	Joback Method
cpg	240.59	J/mol×K	595.78	Joback Method
cpg	233.34	J/mol×K	562.97	Joback Method
cpg	225.76	J/mol×K	530.15	Joback Method
cpg	217.82	J/mol×K	497.33	Joback Method
cpg	254.06	J/mol×K	661.42	Joback Method
dvisc	0.0003158	Pa×s	464.51	Joback Method
dvisc	0.0004081	Pa×s	430.94	Joback Method
dvisc	0.0005509	Pa×s	397.38	Joback Method
dvisc	0.0007858	Pa×s	363.81	Joback Method
dvisc	0.0012050	Pa×s	330.24	Joback Method
dvisc	0.0020352	Pa×s	296.68	Joback Method
dvisc	0.0039296	Pa×s	263.11	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R30719&Units=SI

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