2,2-Dichloroethyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C7H10Cl2O2/c1-3-5(2)7(10)11-4-6(8)9/h3,6H,4H2,1-2H3/b5-3+
InchiKey: VCAKSASJFAKPJT-HWKANZROSA-N
Formula: C7H10Cl2O2
SMILES: CC=C(C)C(=O)OCC(Cl)Cl
Mol. weight [g/mol]: 197.06

Physical Properties

Property code	Value	Unit	Source
gf	-180.49	kJ/mol	Joback Method
hf	-361.94	kJ/mol	Joback Method
hfus	20.44	kJ/mol	Joback Method
hvap	48.75	kJ/mol	Joback Method
log10ws	-2.38		Crippen Method
logp	2.299		Crippen Method
mcvol	137.110	ml/mol	McGowan Method
pc	2912.39	kPa	Joback Method
rinpol	1241.00		NIST Webbook
tb	514.31	K	Joback Method
tc	719.01	K	Joback Method
tf	266.61	K	Joback Method
vc	0.524	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.62	J/mol×K	514.31	Joback Method
cpg	282.88	J/mol×K	548.43	Joback Method
cpg	292.60	J/mol×K	582.54	Joback Method
cpg	301.78	J/mol×K	616.66	Joback Method
cpg	310.46	J/mol×K	650.78	Joback Method
cpg	318.65	J/mol×K	684.90	Joback Method
cpg	326.37	J/mol×K	719.01	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373735&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
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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume