2-Chloroethyl (E)-2-methylbut-2-enoate

Inchi: InChI=1S/C7H11ClO2/c1-3-6(2)7(9)10-5-4-8/h3H,4-5H2,1-2H3/b6-3+
InchiKey: UTHIRZUMGCPHPR-ZZXKWVIFSA-N
Formula: C7H11ClO2
SMILES: CC=C(C)C(=O)OCCCl
Mol. weight [g/mol]: 162.61

Physical Properties

Property code	Value	Unit	Source
gf	-166.12	kJ/mol	Joback Method
hf	-340.92	kJ/mol	Joback Method
hfus	19.76	kJ/mol	Joback Method
hvap	44.75	kJ/mol	Joback Method
log10ws	-1.62		Crippen Method
logp	1.735		Crippen Method
mcvol	124.870	ml/mol	McGowan Method
pc	3005.73	kPa	Joback Method
rinpol	1159.00		NIST Webbook
rinpol	1159.00		NIST Webbook
tb	477.32	K	Joback Method
tc	672.15	K	Joback Method
tf	251.69	K	Joback Method
vc	0.481	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	248.04	J/mol×K	477.32	Joback Method
cpg	258.54	J/mol×K	509.79	Joback Method
cpg	268.56	J/mol×K	542.26	Joback Method
cpg	278.09	J/mol×K	574.74	Joback Method
cpg	287.17	J/mol×K	607.21	Joback Method
cpg	295.79	J/mol×K	639.68	Joback Method
cpg	303.98	J/mol×K	672.15	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=U373722&Units=SI

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