Isopropenyl chloroformate

Other names: Carbonochloridic acid, 1-methylethenyl ester
Inchi: InChI=1S/C4H5ClO2/c1-3(2)7-4(5)6/h1H2,2H3
InchiKey: AMMGCGVWJMRTQI-UHFFFAOYSA-N
Formula: C4H5ClO2
SMILES: C=C(C)OC(=O)Cl
Mol. weight [g/mol]: 120.53
CAS: 57933-83-2

Physical Properties

Property code	Value	Unit	Source
gf	-183.76	kJ/mol	Joback Method
hf	-270.79	kJ/mol	Joback Method
hfus	10.51	kJ/mol	Joback Method
hvap	37.45	kJ/mol	Joback Method
log10ws	-1.84		Crippen Method
logp	1.895		Crippen Method
mcvol	82.600	ml/mol	McGowan Method
pc	4183.90	kPa	Joback Method
rinpol	694.00		NIST Webbook
tb	401.20	K	Joback Method
tc	596.73	K	Joback Method
tf	221.20	K	Joback Method
vc	0.315	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	136.77	J/mol×K	401.20	Joback Method
cpg	142.91	J/mol×K	433.79	Joback Method
cpg	148.80	J/mol×K	466.38	Joback Method
cpg	154.47	J/mol×K	498.97	Joback Method
cpg	159.91	J/mol×K	531.55	Joback Method
cpg	165.12	J/mol×K	564.14	Joback Method
cpg	170.10	J/mol×K	596.73	Joback Method

Sources

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=C57933832&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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