Methylsulfonic acid, 2,2,2-trichloroethyl ester

Inchi: InChI=1S/C3H5Cl3O3S/c1-10(7,8)9-2-3(4,5)6/h2H2,1H3
InchiKey: WSOBLQNNNMEZAF-UHFFFAOYSA-N
Formula: C3H5Cl3O3S
SMILES: CS(=O)(=O)OCC(Cl)(Cl)Cl
Mol. weight [g/mol]: 227.49

Physical Properties

Property code	Value	Unit	Source
gf	-632.11	kJ/mol	Joback Method
hf	-746.79	kJ/mol	Joback Method
hfus	21.27	kJ/mol	Joback Method
hvap	55.18	kJ/mol	Joback Method
log10ws	-1.55		Crippen Method
logp	1.333		Crippen Method
mcvol	123.810	ml/mol	McGowan Method
pc	4691.31	kPa	Joback Method
rinpol	1280.00		NIST Webbook
rinpol	1280.00		NIST Webbook
tb	447.30	K	Joback Method
tc	646.86	K	Joback Method
tf	276.54	K	Joback Method
vc	0.483	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	215.75	J/mol×K	447.30	Joback Method
cpg	223.31	J/mol×K	480.56	Joback Method
cpg	230.45	J/mol×K	513.82	Joback Method
cpg	237.18	J/mol×K	547.08	Joback Method
cpg	243.49	J/mol×K	580.34	Joback Method
cpg	249.39	J/mol×K	613.60	Joback Method
cpg	254.88	J/mol×K	646.86	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=U354617&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