Methylsulfonic acid, 2,3,4,6-tetrachlorophenyl ester

Inchi: InChI=1S/C7H4Cl4O3S/c1-15(12,13)14-7-4(9)2-3(8)5(10)6(7)11/h2H,1H3
InchiKey: IQBRQZOCZKMQJS-UHFFFAOYSA-N
Formula: C7H4Cl4O3S
SMILES: CS(=O)(=O)Oc1c(Cl)cc(Cl)c(Cl)c1Cl
Mol. weight [g/mol]: 309.98

Physical Properties

Property code	Value	Unit	Source
gf	-539.31	kJ/mol	Joback Method
hf	-645.69	kJ/mol	Joback Method
hfus	35.72	kJ/mol	Joback Method
hvap	74.69	kJ/mol	Joback Method
log10ws	-4.16		Crippen Method
logp	3.639		Crippen Method
mcvol	168.650	ml/mol	McGowan Method
pc	3768.41	kPa	Joback Method
rinpol	2045.00		NIST Webbook
rinpol	2045.00		NIST Webbook
tb	626.08	K	Joback Method
tc	854.07	K	Joback Method
tf	425.62	K	Joback Method
vc	0.659	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	318.51	J/mol×K	626.08	Joback Method
cpg	326.58	J/mol×K	664.08	Joback Method
cpg	334.09	J/mol×K	702.08	Joback Method
cpg	341.02	J/mol×K	740.08	Joback Method
cpg	347.34	J/mol×K	778.07	Joback Method
cpg	353.02	J/mol×K	816.07	Joback Method
cpg	358.03	J/mol×K	854.07	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U354619&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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