Methylsulfonic acid, 2,4,5-trichlorophenyl ester

Inchi: InChI=1S/C7H5Cl3O3S/c1-14(11,12)13-7-3-5(9)4(8)2-6(7)10/h2-3H,1H3
InchiKey: PNZISFJRKQOULX-UHFFFAOYSA-N
Formula: C7H5Cl3O3S
SMILES: CS(=O)(=O)Oc1cc(Cl)c(Cl)cc1Cl
Mol. weight [g/mol]: 275.54

Physical Properties

Property code	Value	Unit	Source
gf	-517.75	kJ/mol	Joback Method
hf	-618.48	kJ/mol	Joback Method
hfus	31.92	kJ/mol	Joback Method
hvap	69.64	kJ/mol	Joback Method
log10ws	-3.47		Crippen Method
logp	2.985		Crippen Method
mcvol	156.410	ml/mol	McGowan Method
pc	4021.02	kPa	Joback Method
rinpol	1841.00		NIST Webbook
tb	583.67	K	Joback Method
tc	807.10	K	Joback Method
tf	383.18	K	Joback Method
vc	0.611	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	299.73	J/mol×K	583.67	Joback Method
cpg	308.73	J/mol×K	620.91	Joback Method
cpg	317.18	J/mol×K	658.15	Joback Method
cpg	325.06	J/mol×K	695.38	Joback Method
cpg	332.35	J/mol×K	732.62	Joback Method
cpg	339.02	J/mol×K	769.86	Joback Method
cpg	345.06	J/mol×K	807.10	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=U354618&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

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