4-Chlorophenylsulfonylacetone

Other names:	p-Chlorophenylsulfonylacetone
	4-Chlorophenylsulfonylpropan-2-one
	Propan-2-one, 1-(4-chlorophenylsulphonyl)-
	4-Chlorobenzenesulphonylpropan-2-one
	1-[(4-Chlorophenyl)sulfonyl]acetone
Inchi:	InChI=1S/C9H9ClO3S/c1-7(11)6-14(12,13)9-4-2-8(10)3-5-9/h2-5H,6H2,1H3
InchiKey:	BRDBHPZILGTBFY-UHFFFAOYSA-N
Formula:	C9H9ClO3S
SMILES:	CC(=O)CS(=O)(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]:	232.68
CAS:	5000-48-6

Physical Properties

Property code	Value	Unit	Source
gf	-481.71	kJ/mol	Joback Method
hf	-585.70	kJ/mol	Joback Method
hfus	29.89	kJ/mol	Joback Method
hvap	68.33	kJ/mol	Joback Method
log10ws	-1.97		Crippen Method
logp	1.703		Crippen Method
mcvol	155.810	ml/mol	McGowan Method
pc	3980.54	kPa	Joback Method
tb	576.06	K	Joback Method
tc	792.00	K	Joback Method
tf	348.54	K	Joback Method
vc	0.613	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	335.62	J/mol×K	576.06	Joback Method
cpg	347.61	J/mol×K	612.05	Joback Method
cpg	358.80	J/mol×K	648.04	Joback Method
cpg	369.22	J/mol×K	684.03	Joback Method

cpg	378.87	J/mol×K	720.02	Joback Method
cpg	387.75	J/mol×K	756.01	Joback Method
cpg	395.88	J/mol×K	792.00	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=C5000486&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
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume