Bis(4-Chlorophenylsulfonyl)methane

Inchi: InChI=1S/C13H10Cl2O4S2/c14-10-1-5-12(6-2-10)20(16,17)9-21(18,19)13-7-3-11(15)4-8
InchiKey: UQLKRAFFXYZVBU-UHFFFAOYSA-N
Formula: C13H10Cl2O4S2
SMILES: O=S(=O)(CS(=O)(=O)c1ccc(Cl)cc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 365.25
CAS: 2394-02-7

Physical Properties

Property code	Value	Unit	Source
gf	-696.80	kJ/mol	Joback Method
hf	-799.71	kJ/mol	Joback Method
hfus	47.88	kJ/mol	Joback Method
hvap	96.45	kJ/mol	Joback Method
log10ws	-3.95		Crippen Method
logp	3.199		Crippen Method
mcvol	227.170	ml/mol	McGowan Method
pc	3916.03	kPa	Joback Method
tb	730.58	K	Joback Method
tc	961.57	K	Joback Method
tf	451.11	K	Joback Method
vc	0.897	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	541.86	J/mol×K	730.58	Joback Method
cpg	554.26	J/mol×K	769.08	Joback Method
cpg	565.37	J/mol×K	807.58	Joback Method
cpg	575.19	J/mol×K	846.07	Joback Method
cpg	583.74	J/mol×K	884.57	Joback Method
cpg	591.04	J/mol×K	923.07	Joback Method
cpg	597.08	J/mol×K	961.57	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=C2394027&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