Benzenesulfonothioic acid, 4-chloro-, S-phenyl ester

Other names: Benzenesulfonic acid, p-chlorothio-, S-phenyl ester
p-Chlorothiolbenzenesulfonic acid, phenyl ester
Inchi: InChI=1S/C12H9ClO2S2/c13-10-6-8-12(9-7-10)17(14,15)16-11-4-2-1-3-5-11/h1-9H
InchiKey: OZBQHMNNLSUKDP-UHFFFAOYSA-N
Formula: C12H9ClO2S2
SMILES: O=S(=O)(Sc1ccccc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 284.78
CAS: 1142-97-8

Physical Properties

Property code	Value	Unit	Source
gf	-182.00	kJ/mol	Joback Method
hf	-256.64	kJ/mol	Joback Method
hfus	34.23	kJ/mol	Joback Method
hvap	77.36	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.821		Crippen Method
mcvol	189.100	ml/mol	McGowan Method
pc	3965.51	kPa	Joback Method
tb	686.29	K	Joback Method
tc	946.53	K	Joback Method
tf	393.24	K	Joback Method
vc	0.721	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	434.60	J/mol×K	686.29	Joback Method
cpg	448.15	J/mol×K	729.66	Joback Method
cpg	460.29	J/mol×K	773.04	Joback Method
cpg	471.07	J/mol×K	816.41	Joback Method
cpg	480.52	J/mol×K	859.78	Joback Method
cpg	488.68	J/mol×K	903.16	Joback Method
cpg	495.58	J/mol×K	946.53	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1142978&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

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