P-chlorobenzene sulfonic acid, 3-chloro-2,6-dimethoxyphenyl ester

Inchi: InChI=1S/C14H12Cl2O5S/c1-19-12-8-7-11(16)13(20-2)14(12)21-22(17,18)10-5-3-9(15)4

InchiKey: LSDAGINLGIKFAD-UHFFFAOYSA-N

Formula: C14H12Cl2O5S

SMILES: COc1ccc(Cl)c(OC)c1OS(=O)(=O)c1ccc(Cl)cc1

Mol. weight [g/mol]: 363.21

CAS: 18092-96-1

Physical Properties

Property code	Value	Unit	Source
gf	-554.10	kJ/mol	Joback Method
hf	-786.60	kJ/mol	Joback Method
hfus	41.88	kJ/mol	Joback Method
hvap	88.59	kJ/mol	Joback Method
log10ws	-4.70		Crippen Method
logp	3.778		Crippen Method
mcvol	230.780	ml/mol	McGowan Method
pc	2684.64	kPa	Joback Method
tb	782.90	K	Joback Method
tc	1011.77	K	Joback Method
tf	515.55	K	Joback Method
vc	0.881	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	581.84	J/mol×K	782.90	Joback Method
cpg	593.96	J/mol×K	821.05	Joback Method
cpg	604.84	J/mol×K	859.19	Joback Method
cpg	614.44	J/mol×K	897.34	Joback Method
cpg	622.73	J/mol×K	935.48	Joback Method
cpg	629.67	J/mol×K	973.63	Joback Method
cpg	635.23	J/mol×K	1011.77	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=C18092961&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