Phenyl p-chloro-benzene sulfonate

Inchi: InChI=1S/C12H9ClO3S/c13-10-6-8-12(9-7-10)17(14,15)16-11-4-2-1-3-5-11/h1-9H
InchiKey: FQIJSBUGQPNMQA-UHFFFAOYSA-N
Formula: C12H9ClO3S
SMILES: O=S(=O)(Oc1ccccc1)c1ccc(Cl)cc1
Mol. weight [g/mol]: 268.72
CAS: 2437-33-4

Physical Properties

Property code	Value	Unit	Source
gf	-320.12	kJ/mol	Joback Method
hf	-430.73	kJ/mol	Joback Method
hfus	31.29	kJ/mol	Joback Method
hvap	72.95	kJ/mol	Joback Method
log10ws	-3.77		Crippen Method
logp	3.108		Crippen Method
mcvol	178.620	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	639.93	K	Joback Method
tc	879.02	K	Joback Method
tf	381.07	K	Joback Method
vc	0.684	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	409.44	J/mol×K	639.93	Joback Method
cpg	423.37	J/mol×K	679.78	Joback Method
cpg	436.13	J/mol×K	719.63	Joback Method
cpg	447.73	J/mol×K	759.48	Joback Method
cpg	458.20	J/mol×K	799.32	Joback Method
cpg	467.55	J/mol×K	839.17	Joback Method
cpg	475.80	J/mol×K	879.02	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2437334&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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