P-chlorophenyl-p-toluenesulfonate

Inchi: InChI=1S/C13H11ClO3S/c1-10-2-8-13(9-3-10)18(15,16)17-12-6-4-11(14)5-7-12/h2-9H,1
InchiKey: PPRVVAPBLOBOSE-UHFFFAOYSA-N
Formula: C13H11ClO3S
SMILES: Cc1ccc(S(=O)(=O)Oc2ccc(Cl)cc2)cc1
Mol. weight [g/mol]: 282.74
CAS: 599-89-3

Physical Properties

Property code	Value	Unit	Source
gf	-321.33	kJ/mol	Joback Method
hf	-462.84	kJ/mol	Joback Method
hfus	33.49	kJ/mol	Joback Method
hvap	75.84	kJ/mol	Joback Method
log10ws	-4.25		Crippen Method
logp	3.416		Crippen Method
mcvol	192.710	ml/mol	McGowan Method
pc	3329.68	kPa	Joback Method
tb	667.79	K	Joback Method
tc	902.87	K	Joback Method
tf	404.86	K	Joback Method
vc	0.741	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	458.18	J/mol×K	667.79	Joback Method
cpg	472.43	J/mol×K	706.97	Joback Method
cpg	485.51	J/mol×K	746.15	Joback Method
cpg	497.43	J/mol×K	785.33	Joback Method
cpg	508.22	J/mol×K	824.51	Joback Method
cpg	517.88	J/mol×K	863.69	Joback Method
cpg	526.42	J/mol×K	902.87	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C599893&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