4-Tert-butylphenyl benzene sulfonate

Inchi: InChI=1S/C16H18O3S/c1-16(2,3)13-9-11-14(12-10-13)19-20(17,18)15-7-5-4-6-8-15/h4-1
InchiKey: GLHUQIUKLSAEEK-UHFFFAOYSA-N
Formula: C16H18O3S
SMILES: CC(C)(C)c1ccc(OS(=O)(=O)c2ccccc2)cc1
Mol. weight [g/mol]: 290.38
CAS: 160788-98-7

Physical Properties

Property code	Value	Unit	Source
gf	-271.67	kJ/mol	Joback Method
hf	-506.30	kJ/mol	Joback Method
hfus	30.04	kJ/mol	Joback Method
hvap	76.17	kJ/mol	Joback Method
log10ws	-4.40		Crippen Method
logp	3.752		Crippen Method
mcvol	222.740	ml/mol	McGowan Method
pc	2629.85	kPa	Joback Method
tb	690.79	K	Joback Method
tc	921.71	K	Joback Method
tf	398.65	K	Joback Method
vc	0.849	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	591.10	J/mol×K	690.79	Joback Method
cpg	608.60	J/mol×K	729.28	Joback Method
cpg	624.66	J/mol×K	767.76	Joback Method
cpg	639.32	J/mol×K	806.25	Joback Method
cpg	652.64	J/mol×K	844.74	Joback Method
cpg	664.67	J/mol×K	883.22	Joback Method
cpg	675.48	J/mol×K	921.71	Joback Method

Sources

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=C160788987&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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