di-p-Tolyl sulfone

Other names:	Bis(4-methylphenyl) sulfone
	Benzene, 1,1'-sulfonylbis(4-methyl-
	p-Tolyl sulfone
	p,p'-Ditolyl sulfone
	Sulfone, di-p-tolyl
	4,4'-Dimethyldiphenylsulfone
	4,4'-Ditolyl sulfone
	Bis(p-tolyl) sulfone
	NSC 208
	di-p-tolyl sulphone
	Benzene, 1,1'-sulfonylbis(4-methyl-)
Inchi:	InChI=1S/C14H14O2S/c1-11-3-7-13(8-4-11)17(15,16)14-9-5-12(2)6-10-14/h3-10H,1-2H3
InchiKey:	WEAYCYAIVOIUMG-UHFFFAOYSA-N
Formula:	C14H14O2S
SMILES:	Cc1ccc(S(=O)(=O)c2ccc(C)cc2)cc1
Mol. weight [g/mol]:	246.32
CAS:	599-66-6

Physical Properties

Property code	Value	Unit	Source
chs	-7800.65 ± 0.50	kJ/mol	NIST Webbook
gf	-195.98	kJ/mol	Joback Method
hf	-202.00 ± 3.00	kJ/mol	NIST Webbook
hfs	-311.40 ± 0.80	kJ/mol	NIST Webbook
hfus	30.70	kJ/mol	Joback Method
hsub	110.00 ± 2.00	kJ/mol	NIST Webbook
hvap	71.27	kJ/mol	Joback Method
ie	8.66 ± 0.04	eV	NIST Webbook
log10ws	-3.79		Crippen Method
logp	3.136		Crippen Method
mcvol	188.690	ml/mol	McGowan Method
pc	3173.97	kPa	Joback Method
tb	630.82	K	Joback Method
tc	861.63	K	Joback Method
tf	429.00 ± 3.00	K	NIST Webbook
tf	421.90 ± 1.50	K	NIST Webbook
vc	0.730	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	456.66	J/mol×K	630.82	Joback Method
cpg	473.14	J/mol×K	669.29	Joback Method
cpg	488.39	J/mol×K	707.76	Joback Method
cpg	502.46	J/mol×K	746.22	Joback Method
cpg	515.36	J/mol×K	784.69	Joback Method
cpg	527.14	J/mol×K	823.16	Joback Method
cpg	537.83	J/mol×K	861.63	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C599666&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

chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
gf: Standard Gibbs free energy of formation
hf: Enthalpy of formation at standard conditions
hfs: Solid phase enthalpy of formation at standard conditions
hfus: Enthalpy of fusion at standard conditions
hsub: Enthalpy of sublimation at standard conditions
hvap: Enthalpy of vaporization at standard conditions
ie: Ionization energy
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