Benzene, 1-methyl-4-(phenylsulfonyl)-

Other names:	Sulfone, phenyl p-tolyl
	Phenyl p-tolyl sulfone
	4-Methyldiphenyl sulfone
	p-(phenylsulphonyl)toluene
Inchi:	InChI=1S/C13H12O2S/c1-11-7-9-13(10-8-11)16(14,15)12-5-3-2-4-6-12/h2-10H,1H3
InchiKey:	YBRXHRWLEFCFEG-UHFFFAOYSA-N
Formula:	C13H12O2S
SMILES:	Cc1ccc(S(=O)(=O)c2ccccc2)cc1
Mol. weight [g/mol]:	232.30
CAS:	640-57-3

Physical Properties

Property code	Value	Unit	Source
gf	-194.77	kJ/mol	Joback Method
hf	-303.41	kJ/mol	Joback Method
hfus	28.50	kJ/mol	Joback Method
hvap	68.38	kJ/mol	Joback Method
log10ws	-3.31		Crippen Method
logp	2.828		Crippen Method
mcvol	174.600	ml/mol	McGowan Method
pc	3611.55	kPa	Joback Method
tb	602.96	K	Joback Method
tc	837.49	K	Joback Method
tf	395.00 ± 2.00	K	NIST Webbook
tf	400.40 ± 1.50	K	NIST Webbook
vc	0.673	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	407.39	J/mol×K	602.96	Joback Method
cpg	423.63	J/mol×K	642.05	Joback Method
cpg	438.62	J/mol×K	681.14	Joback Method
cpg	452.41	J/mol×K	720.23	Joback Method

cpg	465.02	J/mol×K	759.31	Joback Method
cpg	476.50	J/mol×K	798.40	Joback Method
cpg	486.88	J/mol×K	837.49	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C640573&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