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

Other names:	(p-Tolylsulfonyl)methane
	1-Methansulfonyl-4-methylbenzene
	1-Methyl-4-(methyl-sulphonyl)benzene
	1-methyl-4-(methylsulfonyl)benzene
	4-methylphenyl methyl sulfone
	4-methylsulfonyltoluene
	Methyl p-tolyl sulphone
	NSC 2722
	NSC 29038
	Sulfone, methyl p-tolyl
	methyl 4-tolyl sulfone
	methyl p-tolyl sulfone
	p-(methylsulphonyl)toluene
	p-Tolyl methyl sulfone
Inchi:	InChI=1S/C8H10O2S/c1-7-3-5-8(6-4-7)11(2,9)10/h3-6H,1-2H3
InchiKey:	YYDNBUBMBZRNQQ-UHFFFAOYSA-N
Formula:	C8H10O2S
SMILES:	Cc1ccc(S(C)(=O)=O)cc1
Mol. weight [g/mol]:	170.23
CAS:	3185-99-7

Physical Properties

Property code	Value	Unit	Source
chl	-4806.45 ± 0.54	kJ/mol	NIST Webbook
gf	-349.28	kJ/mol	Joback Method
hf	-273.10 ± 3.40	kJ/mol	NIST Webbook
hfl	-373.10 ± 0.79	kJ/mol	NIST Webbook
hfus	21.51	kJ/mol	Joback Method
hvap	90.00 ± 2.00	kJ/mol	NIST Webbook
log10ws	-1.64		Crippen Method
logp	1.399		Crippen Method
mcvol	127.910	ml/mol	McGowan Method
pc	4356.87	kPa	Joback Method
tb	461.88	K	Joback Method
tc	666.86	K	Joback Method

tf	359.55	K	Thermodynamic functions of 1-methyl-4-(methylsulfonyl)benzene solubility in nine organic solvents from T = (278.15 to 318.15) K
vc	0.501	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	249.63	J/mol×K	461.88	Joback Method
cpg	262.50	J/mol×K	496.04	Joback Method
cpg	274.73	J/mol×K	530.21	Joback Method
cpg	286.31	J/mol×K	564.37	Joback Method
cpg	297.25	J/mol×K	598.53	Joback Method
cpg	307.56	J/mol×K	632.70	Joback Method
cpg	317.24	J/mol×K	666.86	Joback Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Thermodynamic functions of 1-methyl-4-(methylsulfonyl)benzene solubility in nine organic solvents from T = (278.15 to 318.15) K:	https://www.doi.org/10.1016/j.jct.2016.08.021
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=C3185997&Units=SI

Legend

chl:	Standard liquid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfl:	Liquid phase 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