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

Other names:	Anisole, p-(methylsulfonyl)-
	p-(Methylsulfonyl)anisole
	p-Anisyl methyl sulfone
	p-Methoxyphenyl methyl sulfone
	Methyl 4-methoxyphenyl sulfone
	4-Methoxyphenyl methyl sulfone
Inchi:	InChI=1S/C8H10O3S/c1-11-7-3-5-8(6-4-7)12(2,9)10/h3-6H,1-2H3
InchiKey:	KAZUCVUGWMQGMC-UHFFFAOYSA-N
Formula:	C8H10O3S
SMILES:	COc1ccc(S(C)(=O)=O)cc1
Mol. weight [g/mol]:	186.23
CAS:	3517-90-6

Physical Properties

Property code	Value	Unit	Source
gf	-454.28	kJ/mol	Joback Method
hf	-568.96	kJ/mol	Joback Method
hfus	22.69	kJ/mol	Joback Method
hvap	57.39	kJ/mol	Joback Method
log10ws	-1.28		Crippen Method
logp	1.099		Crippen Method
mcvol	133.780	ml/mol	McGowan Method
pc	4260.71	kPa	Joback Method
tb	484.30	K	Joback Method
tc	687.75	K	Joback Method
tf	279.65	K	Joback Method
vc	0.519	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	272.85	J/mol×K	484.30	Joback Method
cpg	285.44	J/mol×K	518.21	Joback Method
cpg	297.45	J/mol×K	552.12	Joback Method

cpg	308.87	J/mol×K	586.03	Joback Method
cpg	319.70	J/mol×K	619.93	Joback Method
cpg	329.94	J/mol×K	653.84	Joback Method
cpg	339.56	J/mol×K	687.75	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3517906&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