Benzene, (methylsulfinyl)-

Other names:	Sulfoxide, methyl phenyl
	(Methylsulfinyl)benzene
	Methyl phenyl sulfoxide
	Phenyl methyl sulfoxide
	Thioanisole S-oxide
	(methylsulphinyl)benzene
Inchi:	InChI=1S/C7H8OS/c1-9(8)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	JXTGICXCHWMCPM-UHFFFAOYSA-N
Formula:	C7H8OS
SMILES:	CS(=O)c1ccccc1
Mol. weight [g/mol]:	140.20
CAS:	1193-82-4

Physical Properties

Property code	Value	Unit	Source
gf	-97.24	kJ/mol	Joback Method
hf	-157.02	kJ/mol	Joback Method
hfus	15.68	kJ/mol	Joback Method
hvap	46.18	kJ/mol	Joback Method
ie	8.85	eV	NIST Webbook
ie	8.79	eV	NIST Webbook
log10ws	-0.97		Crippen Method
logp	1.424		Crippen Method
mcvol	107.950	ml/mol	McGowan Method
pc	4608.87	kPa	Joback Method
tb	444.52	K	Joback Method
tc	666.33	K	Joback Method
tf	231.55	K	Joback Method
vc	0.409	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	195.82	J/mol×K	444.52	Joback Method

cpg	207.91	J/mol×K	481.49	Joback Method
cpg	219.29	J/mol×K	518.46	Joback Method
cpg	229.97	J/mol×K	555.43	Joback Method
cpg	239.98	J/mol×K	592.39	Joback Method
cpg	249.32	J/mol×K	629.36	Joback Method
cpg	258.02	J/mol×K	666.33	Joback Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1193824&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
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