Sulfone, methyl phenyl

Other names:	Benzene, (methylsulfonyl)-
	Methyl phenyl sulfone
	Phenyl methyl sulfone
	(Methylsulphonyl)benzene
	Methyl phenyl sulphone
	(Phenylsulfonyl)methane
	(Methylsulfonyl)benzene
	NSC 41587
Inchi:	InChI=1S/C7H8O2S/c1-10(8,9)7-5-3-2-4-6-7/h2-6H,1H3
InchiKey:	JCDWETOKTFWTHA-UHFFFAOYSA-N
Formula:	C7H8O2S
SMILES:	CS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	156.20
CAS:	3112-85-4

Physical Properties

Property code	Value	Unit	Source
affp	812.70	kJ/mol	NIST Webbook
basg	780.30	kJ/mol	NIST Webbook
chl	-4154.80 ± 0.67	kJ/mol	NIST Webbook
gf	-348.07	kJ/mol	Joback Method
hf	-253.40 ± 3.10	kJ/mol	NIST Webbook
hfl	-345.40 ± 0.88	kJ/mol	NIST Webbook
hfus	19.30	kJ/mol	Joback Method
hvap	52.09	kJ/mol	Joback Method
ie	9.50	eV	NIST Webbook
ie	9.85	eV	NIST Webbook
ie	9.74	eV	NIST Webbook
log10ws	-1.17		Crippen Method
logp	1.090		Crippen Method
mcvol	113.820	ml/mol	McGowan Method
pc	5073.01	kPa	Joback Method
tb	434.02	K	Joback Method
tc	640.17	K	Joback Method
tf	361.00 ± 3.00	K	NIST Webbook
tf	359.00 ± 3.00	K	NIST Webbook
tf	360.00 ± 3.00	K	NIST Webbook

tf	363.00 ± 2.00	K	NIST Webbook
tf	358.00 ± 2.00	K	NIST Webbook
vc	0.446	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	208.52	J/mol×K	434.02	Joback Method
cpg	220.66	J/mol×K	468.38	Joback Method
cpg	232.16	J/mol×K	502.74	Joback Method
cpg	243.01	J/mol×K	537.10	Joback Method
cpg	253.24	J/mol×K	571.45	Joback Method
cpg	262.84	J/mol×K	605.81	Joback Method
cpg	271.83	J/mol×K	640.17	Joback Method

Sources

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
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C3112854&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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
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