Sulfone, methyl styryl

Other names:	Benzene, [2-(methylsulfonyl)ethenyl]-
	Methyl styryl sulfone
	Styryl-methyl-sulfon
	Styryl-methyl-sulfone
Inchi:	InChI=1S/C9H10O2S/c1-12(10,11)8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7+
InchiKey:	RJQJJDKSNFBCFC-BQYQJAHWSA-N
Formula:	C9H10O2S
SMILES:	CS(=O)(=O)C=Cc1ccccc1
Mol. weight [g/mol]:	182.24
CAS:	5342-84-7

Physical Properties

Property code	Value	Unit	Source
gf	-251.01	kJ/mol	Joback Method
hf	-328.69	kJ/mol	Joback Method
hfus	24.69	kJ/mol	Joback Method
hvap	56.50	kJ/mol	Joback Method
ie	8.70	eV	NIST Webbook
ie	9.08	eV	NIST Webbook
log10ws	-2.04		Crippen Method
logp	1.702		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	4194.74	kPa	Joback Method
tb	483.94	K	Joback Method
tc	694.78	K	Joback Method
tf	251.09	K	Joback Method
vc	0.537	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.54	J/mol×K	483.94	Joback Method
cpg	288.47	J/mol×K	519.08	Joback Method
cpg	301.54	J/mol×K	554.22	Joback Method

cpg	313.76	J/mol×K	589.36	Joback Method
cpg	325.18	J/mol×K	624.50	Joback Method
cpg	335.81	J/mol×K	659.64	Joback Method
cpg	345.69	J/mol×K	694.78	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=C5342847&Units=SI

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