2-(p-Methoxyphenyl)vinylmethylsulfone

Other names: Benzene, 1-methoxy-4-[2-(methylsulfonyl)ethenyl]-
4-Methoxystyryl-methyl-sulfon
4-Methoxystyryl-methyl-sulfone
Inchi: InChI=1S/C10H12O3S/c1-13-10-5-3-9(4-6-10)7-8-14(2,11)12/h3-8H,1-2H3/b8-7+
InchiKey: ASRRXCMJEGWVQS-BQYQJAHWSA-N
Formula: C10H12O3S
SMILES: COc1ccc(C=CS(C)(=O)=O)cc1
Mol. weight [g/mol]: 212.26
CAS: 70784-98-4

Physical Properties

Property code	Value	Unit	Source
gf	-357.22	kJ/mol	Joback Method
hf	-493.02	kJ/mol	Joback Method
hfus	28.08	kJ/mol	Joback Method
hvap	61.80	kJ/mol	Joback Method
ie	8.52	eV	NIST Webbook
log10ws	-2.16		Crippen Method
logp	1.711		Crippen Method
mcvol	157.660	ml/mol	McGowan Method
pc	3577.07	kPa	Joback Method
tb	534.22	K	Joback Method
tc	741.12	K	Joback Method
tf	297.11	K	Joback Method
vc	0.612	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	343.26	J/mol×K	534.22	Joback Method
cpg	357.34	J/mol×K	568.70	Joback Method
cpg	370.65	J/mol×K	603.19	Joback Method
cpg	383.19	J/mol×K	637.67	Joback Method
cpg	394.97	J/mol×K	672.15	Joback Method

cpg	406.00	J/mol×K	706.63	Joback Method
cpg	416.29	J/mol×K	741.12	Joback Method

Sources

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=C70784984&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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