Benzene, 1-(ethenylsulfonyl)-4-methyl-

Other names:	Sulfone, p-tolyl vinyl
	p-Tolyl vinyl sulfone
	p-Tosylethylene
	4-Methylphenyl vinyl sulfone
Inchi:	InChI=1S/C9H10O2S/c1-3-12(10,11)9-6-4-8(2)5-7-9/h3-7H,1H2,2H3
InchiKey:	VZQFRPMWVXCURA-UHFFFAOYSA-N
Formula:	C9H10O2S
SMILES:	C=CS(=O)(=O)c1ccc(C)cc1
Mol. weight [g/mol]:	182.24
CAS:	5535-52-4

Physical Properties

Property code	Value	Unit	Source
chs	-5328.40 ± 3.00	kJ/mol	NIST Webbook
gf	-253.02	kJ/mol	Joback Method
hf	-162.00 ± 4.20	kJ/mol	NIST Webbook
hfs	-244.40 ± 3.10	kJ/mol	NIST Webbook
hfus	22.82	kJ/mol	Joback Method
hsub	82.00 ± 2.00	kJ/mol	NIST Webbook
hvap	56.53	kJ/mol	Joback Method
log10ws	-2.41		Crippen Method
logp	1.912		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	4062.13	kPa	Joback Method
tb	481.44	K	Joback Method
tc	688.13	K	Joback Method
tf	266.93	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.63	J/mol×K	481.44	Joback Method
cpg	287.91	J/mol×K	515.89	Joback Method

cpg	300.46	J/mol×K	550.34	Joback Method
cpg	312.29	J/mol×K	584.78	Joback Method
cpg	323.42	J/mol×K	619.23	Joback Method
cpg	333.84	J/mol×K	653.68	Joback Method
cpg	343.59	J/mol×K	688.13	Joback Method
hfust	10.88	kJ/mol	340.40	NIST Webbook

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=C5535524&Units=SI

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hsub:	Enthalpy of sublimation 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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.