(1,2-Propadienylsulphonyl)-benzene

Inchi: InChI=1S/C9H8O2S/c1-2-8-12(10,11)9-6-4-3-5-7-9/h3-8H,1H2
InchiKey: PVMCSDIRNOOAJI-UHFFFAOYSA-N
Formula: C9H8O2S
SMILES: C=C=CS(=O)(=O)c1ccccc1
Mol. weight [g/mol]: 180.22
CAS: 2525-42-0

Physical Properties

Property code	Value	Unit	Source
chs	-5183.60 ± 4.90	kJ/mol	NIST Webbook
gf	-115.11	kJ/mol	Joback Method
hf	2.10 ± 5.90	kJ/mol	NIST Webbook
hfs	-103.40 ± 5.00	kJ/mol	NIST Webbook
hfus	25.34	kJ/mol	Joback Method
hsub	105.00 ± 3.00	kJ/mol	NIST Webbook
hvap	56.30	kJ/mol	Joback Method
log10ws	-2.23		Crippen Method
logp	1.759		Crippen Method
mcvol	133.400	ml/mol	McGowan Method
pc	4678.49	kPa	Joback Method
tb	479.73	K	Joback Method
tc	698.01	K	Joback Method
tf	260.92	K	Joback Method
vc	0.518	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	260.43	J/mol×K	479.73	Joback Method
cpg	273.35	J/mol×K	516.11	Joback Method
cpg	285.53	J/mol×K	552.49	Joback Method
cpg	296.99	J/mol×K	588.87	Joback Method
cpg	307.71	J/mol×K	625.25	Joback Method
cpg	317.72	J/mol×K	661.63	Joback Method

cpg	327.00	J/mol×K	698.01	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C2525420&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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

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
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