Allylphenyl sulfone

Other names:	Benzene, (2-propenylsulfonyl)-
	Sulfone, allyl phenyl
	Phenyl allyl sulfone
	(allylsulphonyl)benzene
Inchi:	InChI=1S/C9H10O2S/c1-2-8-12(10,11)9-6-4-3-5-7-9/h2-7H,1,8H2
InchiKey:	KYPIULIVYSQNNT-UHFFFAOYSA-N
Formula:	C9H10O2S
SMILES:	C=CCS(=O)(=O)c1ccccc1
Mol. weight [g/mol]:	182.24
CAS:	16212-05-8

Physical Properties

Property code	Value	Unit	Source
gf	-243.39	kJ/mol	Joback Method
hf	-320.48	kJ/mol	Joback Method
hfus	23.20	kJ/mol	Joback Method
hvap	55.87	kJ/mol	Joback Method
log10ws	-1.86		Crippen Method
logp	1.646		Crippen Method
mcvol	137.700	ml/mol	McGowan Method
pc	4140.93	kPa	Joback Method
tb	476.46	K	Joback Method
tc	681.88	K	Joback Method
tf	254.41	K	Joback Method
vc	0.538	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	274.16	J/mol×K	476.46	Joback Method
cpg	287.87	J/mol×K	510.70	Joback Method
cpg	300.78	J/mol×K	544.93	Joback Method
cpg	312.91	J/mol×K	579.17	Joback Method
cpg	324.29	J/mol×K	613.41	Joback Method

cpg	334.93	J/mol×K	647.64	Joback Method
cpg	344.85	J/mol×K	681.88	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C16212058&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

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
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

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