Allylphenyl sulfide

Other names:	(Allylthio)benzene
	Benzene, (2-propenylthio)-
	3-(Phenylthio)propene
	3-(Phenylthio)prop-1-ene
	Sulfide, allyl phenyl
	Allyl phenyl thioether
	Phenyl allyl thioether
	Phenyl allyl sulfide
Inchi:	InChI=1S/C9H10S/c1-2-8-10-9-6-4-3-5-7-9/h2-7H,1,8H2
InchiKey:	QGNRLAFFKKBSIM-UHFFFAOYSA-N
Formula:	C9H10S
SMILES:	C=CCSc1ccccc1
Mol. weight [g/mol]:	150.24
CAS:	5296-64-0

Physical Properties

Property code	Value	Unit	Source
gf	258.27	kJ/mol	Joback Method
hf	174.74	kJ/mol	Joback Method
hfus	15.96	kJ/mol	Joback Method
hvap	44.05	kJ/mol	Joback Method
ie	7.91 ± 0.01	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.965		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3493.01	kPa	Joback Method
tb	497.46	K	Joback Method
tc	733.42	K	Joback Method
tf	250.25	K	Joback Method
vc	0.467	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cpg	247.62	J/mol×K	497.46	Joback Method
cpg	261.28	J/mol×K	536.79	Joback Method
cpg	274.02	J/mol×K	576.11	Joback Method
cpg	285.86	J/mol×K	615.44	Joback Method
cpg	296.85	J/mol×K	654.77	Joback Method
cpg	307.04	J/mol×K	694.09	Joback Method
cpg	316.46	J/mol×K	733.42	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=C5296640&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