Phenyl propargyl sulfide

Other names: Phenyl propargyl sulphide
Inchi: InChI=1S/C9H8S/c1-2-8-10-9-6-4-3-5-7-9/h1,3-7H,8H2
InchiKey: HXKVNRKJSSHQQY-UHFFFAOYSA-N
Formula: C9H8S
SMILES: C#CCSc1ccccc1
Mol. weight [g/mol]: 148.22
CAS: 5651-88-7

Physical Properties

Property code	Value	Unit	Source
gf	393.50	kJ/mol	Joback Method
hf	341.21	kJ/mol	Joback Method
hfus	20.21	kJ/mol	Joback Method
hvap	44.58	kJ/mol	Joback Method
log10ws	-2.85		Crippen Method
logp	2.412		Crippen Method
mcvol	121.660	ml/mol	McGowan Method
pc	3975.52	kPa	Joback Method
tb	490.90	K	Joback Method
tc	740.00	K	Joback Method
tf	298.98	K	Joback Method
vc	0.448	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	232.36	J/mol×K	490.90	Joback Method
cpg	245.03	J/mol×K	532.42	Joback Method
cpg	256.76	J/mol×K	573.93	Joback Method
cpg	267.60	J/mol×K	615.45	Joback Method
cpg	277.59	J/mol×K	656.97	Joback Method
cpg	286.78	J/mol×K	698.48	Joback Method
cpg	295.22	J/mol×K	740.00	Joback Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5651887&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

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