Benzene, (ethenylthio)-

Other names:	Phenylthioethene
	Phenylthioethylene
	Phenyl vinyl sulfide
	Phenyl vinyl thioether
	Sulfide, phenyl vinyl
	Vinyl phenyl sulfide
	Vinylthiobenzene
	(Vinylsulfanyl)benzene
	(Ethenylthio)benzene
	Phenyl vinyl sulphide
Inchi:	InChI=1S/C8H8S/c1-2-9-8-6-4-3-5-7-8/h2-7H,1H2
InchiKey:	GMPDOIGGGXSAPL-UHFFFAOYSA-N
Formula:	C8H8S
SMILES:	C=CSc1ccccc1
Mol. weight [g/mol]:	136.21
CAS:	1822-73-7

Physical Properties

Property code	Value	Unit	Source
gf	249.85	kJ/mol	Joback Method
hf	195.38	kJ/mol	Joback Method
hfus	13.37	kJ/mol	Joback Method
hvap	41.83	kJ/mol	Joback Method
ie	7.96 ± 0.01	eV	NIST Webbook
log10ws	-2.98		Crippen Method
logp	2.922		Crippen Method
mcvol	111.870	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
rinpol	1141.00		NIST Webbook
rinpol	1141.00		NIST Webbook
tb	474.58	K	Joback Method
tc	714.89	K	Joback Method
tf	238.98	K	Joback Method
vc	0.410	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	206.03	J/mol×K	474.58	Joback Method
cpg	218.51	J/mol×K	514.63	Joback Method
cpg	230.11	J/mol×K	554.68	Joback Method
cpg	240.88	J/mol×K	594.74	Joback Method
cpg	250.85	J/mol×K	634.79	Joback Method
cpg	260.07	J/mol×K	674.84	Joback Method
cpg	268.56	J/mol×K	714.89	Joback Method

Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	367.70	K	3.30	NIST Webbook

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=C1822737&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
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tbrp:	Boiling point at reduced pressure
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume