

Benzene, (ethenylsulfinyl)-

Other names:	Phenyl vinyl sulfoxide Sulfoxide, phenyl vinyl phenyl vinyl sulphoxide
Inchi:	InChI=1S/C8H8OS/c1-2-10(9)8-6-4-3-5-7-8/h2-7H,1H2
InchiKey:	MZMJHXYLRTLQX-UHFFFAOYSA-N
Formula:	C8H8OS
SMILES:	C=CS(=O)c1ccccc1
Mol. weight [g/mol]:	152.21
CAS:	20451-53-0

Physical Properties

Property code	Value	Unit	Source
gf	-0.98	kJ/mol	Joback Method
hf	-52.23	kJ/mol	Joback Method
hfus	16.99	kJ/mol	Joback Method
hvap	47.73	kJ/mol	Joback Method
log10ws	-1.73		Crippen Method
logp	1.938		Crippen Method
mcvol	117.740	ml/mol	McGowan Method
pc	4288.66	kPa	Joback Method
tb	464.08	K	Joback Method
tc	687.70	K	Joback Method
tf	241.06	K	Joback Method
vc	0.447	m ³ /kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	219.48	J/mol×K	464.08	Joback Method
cpg	232.06	J/mol×K	501.35	Joback Method
cpg	243.84	J/mol×K	538.62	Joback Method
cpg	254.83	J/mol×K	575.89	Joback Method
cpg	265.07	J/mol×K	613.16	Joback Method
cpg	274.58	J/mol×K	650.43	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C20451530&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
mccvol:	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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