Benzene,[2-(methylthio)ethenyl]-(Z)-

Inchi: InChI=1S/C9H10S/c1-10-8-7-9-5-3-2-4-6-9/h2-8H,1H3/b8-7-
InchiKey: BWRWWBWZSDMTFX-FPLPWBNLSA-N
Formula: C9H10S
SMILES: CSC=Cc1ccccc1
Mol. weight [g/mol]: 150.24
CAS: 35822-50-5

Physical Properties

Property code	Value	Unit	Source
gf	250.65	kJ/mol	Joback Method
hf	166.53	kJ/mol	Joback Method
hfus	17.44	kJ/mol	Joback Method
hvap	44.68	kJ/mol	Joback Method
ie	7.75	eV	NIST Webbook
ie	8.75	eV	NIST Webbook
log10ws	-3.09		Crippen Method
logp	3.020		Crippen Method
mcvol	125.960	ml/mol	McGowan Method
pc	3534.66	kPa	Joback Method
tb	504.94	K	Joback Method
tc	747.08	K	Joback Method
tf	246.93	K	Joback Method
vc	0.466	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	247.64	J/mol×K	504.94	Joback Method
cpg	261.50	J/mol×K	545.30	Joback Method
cpg	274.35	J/mol×K	585.65	Joback Method
cpg	286.25	J/mol×K	626.01	Joback Method
cpg	297.25	J/mol×K	666.37	Joback Method
cpg	307.41	J/mol×K	706.73	Joback Method
cpg	316.79	J/mol×K	747.08	Joback Method

Sources

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=C35822505&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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