Sulfine

Inchi: InChI=1S/CH2OS/c1-3-2/h1H2
InchiKey: IWOKCMBOJXYDEE-UHFFFAOYSA-N
Formula: CH2OS
SMILES: C=S=O
Mol. weight [g/mol]: 62.09
CAS: 40100-16-1

Physical Properties

Property code	Value	Unit	Source
affp	798.90	kJ/mol	NIST Webbook
affp	787.60 ± 2.60	kJ/mol	NIST Webbook
affp	787.60 ± 2.60	kJ/mol	NIST Webbook
basg	755.10 ± 1.50	kJ/mol	NIST Webbook
basg	755.10 ± 1.50	kJ/mol	NIST Webbook
basg	766.40	kJ/mol	NIST Webbook
gf	-160.06	kJ/mol	Joback Method
hf	-147.08	kJ/mol	Joback Method
hfus	6.40	kJ/mol	Joback Method
hvap	29.75	kJ/mol	Joback Method
log10ws	0.65		Crippen Method
logp	-0.369		Crippen Method
mcvol	42.870	ml/mol	McGowan Method
pc	7330.17	kPa	Joback Method
tb	274.46	K	Joback Method
tc	443.55	K	Joback Method
tf	154.66	K	Joback Method
vc	0.164	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	51.79	J/mol×K	274.46	Joback Method
cpg	54.73	J/mol×K	302.64	Joback Method
cpg	57.49	J/mol×K	330.82	Joback Method

cpg	60.08	J/mol×K	359.00	Joback Method
cpg	62.51	J/mol×K	387.19	Joback Method
cpg	64.77	J/mol×K	415.37	Joback Method
cpg	66.89	J/mol×K	443.55	Joback Method

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C40100161&Units=SI

Legend

affp: Proton affinity
basg: Gas basicity
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