Thioformaldehyde

Inchi: InChI=1S/CH2S/c1-2/h1H2
InchiKey: DBTDEFJAFBUGPP-UHFFFAOYSA-N
Formula: CH2S
SMILES: C=S
Mol. weight [g/mol]: 46.09
CAS: 865-36-1

Physical Properties

Property code	Value	Unit	Source
affp	759.70	kJ/mol	NIST Webbook
basg	730.50	kJ/mol	NIST Webbook
ea	0.47 ± 0.02	eV	NIST Webbook
gf	90.77	kJ/mol	Joback Method
hf	90.00 ± 8.00	kJ/mol	NIST Webbook
hf	118.00 ± 8.40	kJ/mol	NIST Webbook
hfus	2.78	kJ/mol	Joback Method
hvap	23.84	kJ/mol	Joback Method
ie	9.34 ± 0.01	eV	NIST Webbook
ie	9.44 ± 0.05	eV	NIST Webbook
ie	9.00	eV	NIST Webbook
ie	9.33	eV	NIST Webbook
ie	9.38 ± 0.00	eV	NIST Webbook
ie	9.38	eV	NIST Webbook
log10ws	-0.60		Crippen Method
logp	0.616		Crippen Method
mcvol	37.000	ml/mol	McGowan Method
pc	6535.23	kPa	Joback Method
tb	284.96	K	Joback Method
tc	470.35	K	Joback Method
tf	152.58	K	Joback Method
vc	0.128	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	39.88	J/mol×K	284.96	Joback Method
cpg	42.33	J/mol×K	315.86	Joback Method
cpg	44.58	J/mol×K	346.76	Joback Method
cpg	46.63	J/mol×K	377.65	Joback Method
cpg	48.51	J/mol×K	408.55	Joback Method
cpg	50.22	J/mol×K	439.45	Joback Method
cpg	51.77	J/mol×K	470.35	Joback Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C865361&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

affp: Proton affinity
basg: Gas basicity
cpg: Ideal gas heat capacity
ea: Electron affinity
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

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