Methanesulfinic acid

Inchi: InChI=1S/CH4O2S/c1-4(2)3/h1H3,(H,2,3)
InchiKey: XNEFVTBPCXGIRX-UHFFFAOYSA-N
Formula: CH4O2S
SMILES: CS(=O)O
Mol. weight [g/mol]: 80.11
CAS: 17696-73-0

Physical Properties

Property code	Value	Unit	Source
gf	-396.99	kJ/mol	Joback Method
hf	-421.94	kJ/mol	Joback Method
hfus	10.19	kJ/mol	Joback Method
hvap	47.23	kJ/mol	Joback Method
log10ws	0.81		Crippen Method
logp	-0.162		Crippen Method
mcvol	53.040	ml/mol	McGowan Method
pc	7748.96	kPa	Joback Method
tb	372.74	K	Joback Method
tc	547.09	K	Joback Method
tf	198.33	K	Joback Method
vc	0.201	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	85.48	J/mol×K	372.74	Joback Method
cpg	89.11	J/mol×K	401.80	Joback Method
cpg	92.65	J/mol×K	430.86	Joback Method
cpg	96.10	J/mol×K	459.92	Joback Method
cpg	99.46	J/mol×K	488.98	Joback Method
cpg	102.72	J/mol×K	518.04	Joback Method
cpg	105.87	J/mol×K	547.09	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=C17696730&Units=SI

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
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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