Methane disulfonic acid

Other names: methanedisulphonic acid
Inchi: InChI=1S/CH4O6S2/c2-8(3,4)1-9(5,6)7/h1H2,(H,2,3,4)(H,5,6,7)
InchiKey: OPUAWDUYWRUIIL-UHFFFAOYSA-N
Formula: CH4O6S2
SMILES: O=S(=O)(O)CS(=O)(=O)O
Mol. weight [g/mol]: 176.17
CAS: 503-40-2

Physical Properties

Property code	Value	Unit	Source
gf	-1253.18	kJ/mol	Joback Method
hf	-1275.13	kJ/mol	Joback Method
hfus	29.28	kJ/mol	Joback Method
hvap	88.45	kJ/mol	Joback Method
log10ws	0.97		Crippen Method
logp	-1.280		Crippen Method
mcvol	92.870	ml/mol	McGowan Method
pc	14872.10	kPa	Joback Method
tb	502.20	K	Joback Method
tc	659.17	K	Joback Method
tf	299.79	K	Joback Method
vc	0.382	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	193.15	J/mol×K	502.20	Joback Method
cpg	198.13	J/mol×K	528.36	Joback Method
cpg	202.94	J/mol×K	554.52	Joback Method
cpg	207.56	J/mol×K	580.69	Joback Method
cpg	211.98	J/mol×K	606.85	Joback Method
cpg	216.19	J/mol×K	633.01	Joback Method
cpg	220.18	J/mol×K	659.17	Joback Method

Sources

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=C503402&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

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