Methanesulfonic acid

Other names: Methanesulphonic acid
Methylsulfonic acid
Kyselina methansulfonova
CH3SO3H
NSC 3718

Inchi: InChI=1S/CH4O3S/c1-5(2,3)4/h1H3,(H,2,3,4)
InchiKey: AFVFQIVMOAPDHO-UHFFFAOYSA-N
Formula: CH4O3S
SMILES: CS(=O)(=O)O
Mol. weight [g/mol]:   96.11
CAS: 75-75-2

Physical Properties

Property code	Value	Unit	Source
affp	761.30	kJ/mol	NIST Webbook
basg	728.90	kJ/mol	NIST Webbook
gf	-647.82	kJ/mol	Joback Method
hf	-669.55	kJ/mol	Joback Method
hfus	13.81	kJ/mol	Joback Method
hvap	53.13	kJ/mol	Joback Method
log10ws	0.61		Crippen Method
logp	-0.496		Crippen Method
mcvol	58.910	ml/mol	McGowan Method
pc	8783.57	kPa	Joback Method
tb	362.24	K	Joback Method
tc	523.75	K	Joback Method
tf	200.41	K	Joback Method
vc	0.236	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	98.89	J/mol×K	362.24	Joback Method
cpg	102.86	J/mol×K	389.16	Joback Method

cpg	106.75	J/mol×K	416.08	Joback Method
cpg	110.55	J/mol×K	442.99	Joback Method
cpg	114.26	J/mol×K	469.91	Joback Method
cpg	117.86	J/mol×K	496.83	Joback Method
cpg	121.36	J/mol×K	523.75	Joback Method
hvapt	73.90	kJ/mol	417.50	NIST Webbook

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=C75752&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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
hvapt:	Enthalpy of vaporization at a given temperature
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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