

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

Physical Properties

Property code	Value	Unit	Source
affp	761.30	kJ/mol	NIST Webbook
basg	728.90	kJ/mol	NIST Webbook
hf	-567.08	kJ/mol	Cheméo Relay (1.0)
hfus	13.81	kJ/mol	Joback Method
hvap	79.02	kJ/mol	Cheméo Relay (1.0)
ie	11.68	eV	Cheméo Relay (1.0)
logp	-0.496		Crippen Method
mcvol	58.910	ml/mol	McGowan Method
tb	502.56	K	Cheméo Relay (1.0)
tf	397.89	K	Cheméo Relay (1.0)

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

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C75752&Units=SI
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
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
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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