AMINOMETHANESULPHONIC ACID

Other names: Methanesulfonic acid, amino-
(Aminomethyl)sulfonic acid
Aminomethanesulphonic acid
Inchi: InChI=1S/CH5NO3S/c2-1-6(3,4)5/h1-2H2,(H,3,4,5)
InchiKey: OBESRABRARNZJB-UHFFFAOYSA-N
Formula: CH5NO3S
SMILES: NCS(=O)(=O)O
Mol. weight [g/mol]: 111.12

Physical Properties

Property code	Value	Unit	Source
chs	-982.80 ± 1.00	kJ/mol	NIST Webbook
hfs	-727.30 ± 1.10	kJ/mol	NIST Webbook
hfus	19.01	kJ/mol	Joback Method
ie	11.06	eV	Cheméo Relay (1.0)
logp	-1.210		Crippen Method
mcvol	68.890	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	135.49	J/mol×K	434.77	Joback Method
cpg	140.44	J/mol×K	464.17	Joback Method
cpg	145.21	J/mol×K	493.57	Joback Method
cpg	149.81	J/mol×K	522.97	Joback Method
cpg	154.24	J/mol×K	552.37	Joback Method
cpg	158.47	J/mol×K	581.77	Joback Method
cpg	162.51	J/mol×K	611.17	Joback Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C13881919&Units=SI
Joback Method:	https://en.wikipedia.org/wiki/Joback_method
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
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):	

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
hfs:	Solid phase enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
ie:	Ionization energy
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume