

Metanilic acid

Other names: m-Aminobenzenesulfonic acid
Benzenesulfonic acid, 3-amino-
3-Aminobenzenesulphonic acid
m-Anilinesulfonic acid
m-Sulfanilic acid
Aminobenzenesulfonic acid
Kyselina anilin-3-sulfonova
Kyselina metanilova
1-Aminobenzene-3-sulfonic acid
3-Aminobenzenesulfonic acid
Aniline-m-sulfonic acid
3-Sulfoaniline
m-Aminophenylsulfonic acid
NSC 4504

Inchi: InChI=1S/C6H7NO3S/c7-5-2-1-3-6(4-5)11(8,9)10/h1-4H,7H2,(H,8,9,10)
InchiKey: ZAJAQTYSTDTMCU-UHFFFAOYSA-N
Formula: C6H7NO3S
SMILES: Nc1cccc(S(=O)(=O)O)c1
Mol. weight [g/mol]: 173.19
CAS: 121-47-1

Physical Properties

Property code	Value	Unit	Source
chs	-3357.30	kJ/mol	NIST Webbook
gf	-436.49	kJ/mol	Joback Method
hf	-513.90	kJ/mol	Joback Method
hfs	-606.20 ± 1.80	kJ/mol	NIST Webbook
hfus	25.61	kJ/mol	Joback Method
hvap	77.84	kJ/mol	Joback Method
log10ws	-0.69		Crippen Method
logp	0.516		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	7255.44	kPa	Joback Method
tb	580.83	K	Joback Method
tc	787.92	K	Joback Method
tf	378.96	K	Joback Method
vc	0.438	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	261.80	J/mol×K	580.83	Joback Method
cpg	270.63	J/mol×K	615.34	Joback Method
cpg	278.88	J/mol×K	649.86	Joback Method
cpg	286.56	J/mol×K	684.37	Joback Method
cpg	293.68	J/mol×K	718.89	Joback Method
cpg	300.24	J/mol×K	753.40	Joback Method
cpg	306.24	J/mol×K	787.92	Joback Method

Sources

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=C121471&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

chs:	Standard solid enthalpy of combustion
cpg:	Ideal gas heat capacity
gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfs:	Solid phase 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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