3-Aminobenzenesulfonic 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

Physical Properties

Property code	Value	Unit	Source
af	0.7704		Cheméo Relay (1.0)
chs	-3357.30	kJ/mol	NIST Webbook
hf	-424.52	kJ/mol	Cheméo Relay (1.0)
hfs	-606.20 ± 1.80	kJ/mol	NIST Webbook
hfus	25.61	kJ/mol	Joback Method
hvap	109.80	kJ/mol	Cheméo Relay (1.0)
ie	8.64	eV	Cheméo Relay (1.0)
log10ws	-0.16		Cheméo Relay (1.0)
logp	0.516		Crippen Method
mcvol	115.580	ml/mol	McGowan Method
pc	7255.44	kPa	Joback Method
tb	607.04	K	Cheméo Relay (1.0)
tc	910.38	K	Cheméo Relay (1.0)
tf	499.58	K	Cheméo Relay (1.0)

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

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):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C121471&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

af: Acentric Factor
chs: Standard solid enthalpy of combustion
cpg: Ideal gas heat capacity
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
ie: Ionization energy
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