2-Aminobenzothiazole

Other names:	2(3H)-Benzothiazolimine
	2-Aminobenzthiazole
	2-Benzothiazolylamine
	2-Iminobenzothiazoline
	2-aminobenzo[d]thiazole
	2-benzothiazolamine
	Benzothiazol-2-ylamine
	Benzothiazole, 2-amino-
	NSC 4670
	USAF EK-3941
	USAF XR-27
	o-Aminobenzothiazole
Inchi:	InChI=1S/C7H6N2S/c8-7-9-5-3-1-2-4-6(5)10-7/h1-4H,(H2,8,9)
InchiKey:	UHGULLIUJBCTEF-UHFFFAOYSA-N
Formula:	C7H6N2S
SMILES:	Nc1nc2ccccc2s1
Mol. weight [g/mol]:	150.21

Physical Properties

Property code	Value	Unit	Source
ie	8.06	eV	Cheméo Relay (1.0)
log10ws	-2.61		Cheméo Relay (1.0)
logp	1.878		Crippen Method
mcvol	106.880	ml/mol	McGowan Method
tb	544.89	K	Cheméo Relay (1.0)
tf	412.71	K	Cheméo Relay (1.0)

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source

cps	153.21	J/mol×K	298.15	Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry
hvapt	102.10	kJ/mol	298.15	Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches

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):	
Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry:	https://www.doi.org/10.1016/j.jct.2014.01.018
Thermodynamic study of 2-aminothiazole and 2-aminobenzothiazole: Experimental and computational approaches:	https://www.doi.org/10.1016/j.jct.2014.04.001
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C136958&Units=SI

Legend

cps:	Solid phase heat capacity
hvapt:	Enthalpy of vaporization at a given temperature
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point

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