2-Benzothiazolamine, 4-methyl-

Other names:	2-Amino-4-methylbenzothiazole
	2-amino-4-methylbenzo[d]thiazole
	4-methyl-2-aminobenzothiazole
	4-methyl-2-benzothiazolamine
	4-methylbenzothiazol-2-ylamine
	Benzothiazole, 2-amino-4-methyl-
Inchi:	InChI=1S/C8H8N2S/c1-5-3-2-4-6-7(5)10-8(9)11-6/h2-4H,1H3,(H2,9,10)
InchiKey:	GRIATXVEXOFBGO-UHFFFAOYSA-N
Formula:	C8H8N2S
SMILES:	Cc1cccc2sc(N)nc12
Mol. weight [g/mol]:	164.23
CAS:	1477-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.91		Crippen Method
logp	2.187		Crippen Method
mcvol	120.970	ml/mol	McGowan Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cps	182.29	J/mol×K	298.15	Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1477425&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
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
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

cps:	Solid phase heat capacity
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume