

2-Benzothiazolamine, 6-methyl-

Other names:	2-Amino-6-methylbenzothiazole 2-Amino-6-methylbenzthiazol 2-Methylbenzothiazol-2-amine 2-amino-6-methylbenzo[d]thiazole 6-Methyl-2-benzothiazolamine 6-Methyl-benzothiazol-2-ylamine 6-methyl-2-aminobenzothiazole 6-methyl-2-benzothiazolamine Benzothiazole, 2-amino-6-methyl- NSC 118944 NSC 12760 SKF 1045
Inchi:	InChI=1S/C8H8N2S/c1-5-2-3-6-7(4-5)11-8(9)10-6/h2-4H,1H3,(H2,9,10)
InchiKey:	DZWTXWPRWRLHIL-UHFFFAOYSA-N
Formula:	C8H8N2S
SMILES:	<chem>Cc1ccc2nc(N)sc2c1</chem>
Mol. weight [g/mol]:	164.23
CAS:	2536-91-6

Physical Properties

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

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
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cps

197.07

J/mol×K

298.15

Standard enthalpies of formation of 2-aminobenzothiazoles in the crystalline phase by rotating-bomb combustion calorimetry

Sources

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C2536916&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>

Legend

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

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