

2-Amino-5,6-dimethylbenzimidazole

Other names:	1H-Benzimidazol-2-amine, 5,6-dimethyl-Benzimidazole, 2-amino-5,6-dimethyl-5,6-dimethylbenzimidazol-2-ylamine
Inchi:	InChI=1S/C9H11N3/c1-5-3-7-8(4-6(5)2)12-9(10)11-7/h3-4H,1-2H3,(H3,10,11,12)
InchiKey:	YPFQISHSXCFZMU-UHFFFAOYSA-N
Formula:	C9H11N3
SMILES:	Cc1cc2nc(N)[nH]c2cc1C
Mol. weight [g/mol]:	161.20
CAS:	29096-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	1.280		Crippen Method
mcvol	128.690	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C29096751&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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