2-Benzothiazolamine, 4-methoxy-

Other names:	Benzothiazole, 2-amino-4-methoxy- 2-Amino-4-methoxybenzothiazole 4-Methoxy-2-aminobenzothiazole 2-Amino-methoxybenzothiazole 4-Methoxy-1,3-benzothiazol-2-amine 4-methoxybenzothiazol-2-ylamine
Inchi:	InChI=1S/C8H8N2OS/c1-11-5-3-2-4-6-7(5)10-8(9)12-6/h2-4H,1H3,(H2,9,10)
InchiKey:	YEBCRAVYUWNFQT-UHFFFAOYSA-N
Formula:	C8H8N2OS
SMILES:	COc1cccc2sc(N)nc12
Mol. weight [g/mol]:	180.23
CAS:	5464-79-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.887		Crippen Method
mcvol	126.840	ml/mol	McGowan Method
rinpol	1892.00		NIST Webbook
rinpol	1892.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5464799&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l

logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices