

2-Benzothiazolamine, 6-methoxy-

Other names:	Benzothiazole, 2-amino-6-methoxy- 2-Amino-6-methoxybenzothiazole 6-Methoxy-2-aminobenzothiazole 6-Methoxy-2-benzothiazolamine 6-Methoxy-benzothiazol-2-ylamine 6-Methoxy-1,3-benzothiazol-2-amine
Inchi:	InChI=1S/C8H8N2OS/c1-11-5-2-3-6-7(4-5)12-8(9)10-6/h2-4H,1H3,(H2,9,10)
InchiKey:	KZHGPDSVHSDCMX-UHFFFAOYSA-N
Formula:	C8H8N2OS
SMILES:	COc1ccc2nc(N)sc2c1
Mol. weight [g/mol]:	180.23
CAS:	1747-60-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.55		Crippen Method
logp	1.887		Crippen Method
mcpvol	126.840	ml/mol	McGowan Method
rinpol	1888.00		NIST Webbook
rinpol	1888.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1747600&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

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

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