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
mcvol	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/ci990307l

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