5-methoxy-2-methylbenzothiazole

Inchi:	InChI=1S/C9H9NOS/c1-6-10-8-5-7(11-2)3-4-9(8)12-6/h3-5H,1-2H3
InchiKey:	SAQMNBWVOKYKPZ-UHFFFAOYSA-N
Formula:	C9H9NOS
SMILES:	COc1ccc2sc(C)nc2c1
Mol. weight [g/mol]:	179.24
CAS:	2941-69-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.39		Crippen Method
logp	2.613		Crippen Method
mcvol	130.950	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=C2941697&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

Latest version available from:
https://www.chemeo.com/cid/36-404-3/5-methoxy-2-methylbenzothiazole.pdf
Generated by Cheméo on 2024-10-12 07:43:09.075937473 +0000 UTC m=+3299851.712906721.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.