1,2-Benzoisothiazole, 3-methyl

Inchi: InChI=1S/C8H7NS/c1-6-7-4-2-3-5-8(7)9-10-6/h2-5H,1H3
InchiKey: YJRLOOVPHLBHIZ-UHFFFAOYSA-N
Formula: C8H7NS
SMILES: Cc1snc2ccccc12
Mol. weight [g/mol]: 149.21

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.27		Crippen Method
logp	2.605		Crippen Method
mcvol	110.990	ml/mol	McGowan Method
rinpol	1763.00		NIST Webbook
rinpol	1763.00		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=R319989&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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.