2-o-Tolylbenzothiazole

Inchi: InChI=1S/C14H11NS/c1-10-6-2-3-7-11(10)14-15-12-8-4-5-9-13(12)16-14/h2-9H,1H3
InchiKey: AMWVFOHECZHTQT-UHFFFAOYSA-N
Formula: C14H11NS
SMILES: Cc1ccccc1-c1nc2ccccc2s1
Mol. weight [g/mol]: 225.31
CAS: 15903-58-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.88		Crippen Method
logp	4.272		Crippen Method
mcvol	171.770	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=C15903589&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