Benzothiazoline, 2-isopropylidene-3-methyl-

Inchi: InChI=1S/C11H13NS/c1-8(2)11-12(3)9-6-4-5-7-10(9)13-11/h4-7H,1-3H3
InchiKey: JWIINRRTBOURGR-UHFFFAOYSA-N
Formula: C11H13NS
SMILES: CC(C)=C1Sc2ccccc2N1C
Mol. weight [g/mol]: 191.29
CAS: 143268-64-8

Physical Properties

Property code	Value	Unit	Source
ie	6.76	eV	NIST Webbook
log10ws	-3.70		Crippen Method
logp	3.480		Crippen Method
mcvol	153.260	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=C143268648&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

ie: Ionization energy
log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume

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