6-Benzothiazolamine,2-methyl-

Inchi: InChI=1S/C8H8N2S/c1-5-10-7-3-2-6(9)4-8(7)11-5/h2-4H,9H2,1H3
InchiKey: HFUJOSYKJMNSFQ-UHFFFAOYSA-N
Formula: C8H8N2S
SMILES: Cc1nc2ccc(N)cc2s1
Mol. weight [g/mol]: 164.23
CAS: 2941-62-0

Physical Properties

Property code	Value	Unit	Source
ie	7.70	eV	NIST Webbook
log10ws	-2.91		Crippen Method
logp	2.187		Crippen Method
mcvol	120.970	ml/mol	McGowan Method

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=C2941620&Units=SI

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.