

2-Thiazolamine, 4-phenyl-

Other names:	Thiazole, 2-amino-4-phenyl- 2-Amino-4-phenylthiazole 4-Phenyl-2-aminothiazole 4-Phenyl-2-thiazolamine 4-Phenyl-2-thiazolylamine 4-phenylthiazol-2-amine
Inchi:	InChI=1S/C9H8N2S/c10-9-11-8(6-12-9)7-4-2-1-3-5-7/h1-6H,(H2,10,11)
InchiKey:	PYSJLPAOBIGQPK-UHFFFAOYSA-N
Formula:	C9H8N2S
SMILES:	<chem>Nc1nc(-c2ccccc2)cs1</chem>
Mol. weight [g/mol]:	176.24
CAS:	2010-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.23		Crippen Method
logp	2.392		Crippen Method
mcvol	130.760	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=C2010062&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

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