

N-phenyl-1-aziridinecarbothioamide

Inchi:	InChI=1S/C9H10N2S/c12-9(11-6-7-11)10-8-4-2-1-3-5-8/h1-5H,6-7H2,(H,10,12)
InchiKey:	IMRLVMFRZGEAEL-UHFFFAOYSA-N
Formula:	C9H10N2S
SMILES:	S=C(Nc1ccccc1)N1CC1
Mol. weight [g/mol]:	178.25
CAS:	19116-37-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.13		Crippen Method
logp	1.699		Crippen Method
mcvol	135.060	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C19116371&Units=SI

Legend

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

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<https://www.chemeo.com/cid/63-482-7/N-phenyl-1-aziridinecarbothioamide.pdf>

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