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/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=C19116371&Units=SI

Legend

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