

Carbamothioic acid,phenyl-o-(8-methyl-8-azabicyclo[3.2.1]oct-3-y

Inchi:	InChI=1S/C15H20N2OS/c1-17-12-7-8-13(17)10-14(9-12)18-15(19)16-11-5-3-2-4-6-11/h2
InchiKey:	PMWCCSYQQOSQSC-UHFFFAOYSA-N
Formula:	C15H20N2OS
SMILES:	CN1C2CCC1CC(OC(=S)Nc1ccccc1)C2
Mol. weight [g/mol]:	276.40
CAS:	67139-55-3

Physical Properties

Property code	Value	Unit	Source
ie	8.00 ± 0.30	eV	NIST Webbook
log10ws	-3.96		Crippen Method
logp	3.025		Crippen Method
mcvol	214.610	ml/mol	McGowan Method

Sources

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=C67139553&Units=SI&Mask=3FFF
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307I

Legend

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

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