Carbamothioic acid,phenyl-0-(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: 67139-54-2

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: 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=C67139542&Units=SI&Mask=3FFF

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.