

# 3-Quinuclidinone, 2-benzylidene-

**Other names:** 1-Azabicyclo[2.2.2]octan-3-one, 2-(phenylmethylene)-

1-Azabicyclo[2,2,2]octan-3-one, 2-(phenylmethylene)-

**Inchi:** InChI=1S/C14H15NO/c16-14-12-6-8-15(9-7-12)13(14)10-11-4-2-1-3-5-11/h1-5,10,12H,6

**InchiKey:** RBGFDYWXBIXLSF-JLHYYAGUSA-N

**Formula:** C14H15NO

**SMILES:** O=C1C(=Cc2ccccc2)N2CCC1CC2

**Mol. weight [g/mol]:** 213.28

**CAS:** 24123-89-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.70		Crippen Method
logp	2.322		Crippen Method
mcvol	169.890	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](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=C24123895&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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