3-Quinuclidinol

Other names:	1-Azabicyclo[2.2.2]octan-3-ol
	Quinuclidinol
	3-Hydroxyquinuclidine
	Quinuclidinol-3
	3-Hydroxy-1-azabicyclo[2.2.2]octane
	Quinuclidine-3-ol
	Quinuclidin-3-ol
	NSC 93905
Inchi:	InChI=1S/C7H13NO/c9-7-5-8-3-1-6(7)2-4-8/h6-7,9H,1-5H2
InchiKey:	IVLICPVPXWEGCA-UHFFFAOYSA-N
Formula:	C7H13NO
SMILES:	OC1CN2CCC1CC2
Mol. weight [g/mol]:	127.18
CAS:	1619-34-7

Physical Properties

Property code	Value	Unit	Source
ie	8.10	eV	NIST Webbook
log10ws	-0.25		Crippen Method
logp	0.073		Crippen Method
mcvol	103.620	ml/mol	McGowan Method
rinpol	1152.00		NIST Webbook
rinpol	1162.00		NIST Webbook
ripol	1936.20		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	1985.00		NIST Webbook
ripol	2001.00		NIST Webbook

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=C1619347&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices