

1-Azabicyclo[2.2.2]octane-4-methanol

Other names:	4-(Hydroxymethyl)-1-azabicyclo[2.2.2]octane
Inchi:	InChI=1S/C8H15NO/c10-7-8-1-4-9(5-2-8)6-3-8/h10H,1-7H2
InchiKey:	PGGCTNQYCZTVNL-UHFFFAOYSA-N
Formula:	C8H15NO
SMILES:	OCC12CCN(CC1)CC2
Mol. weight [g/mol]:	141.21
CAS:	26608-58-2

Physical Properties

Property code	Value	Unit	Source
ie	8.17 ± 0.01	eV	NIST Webbook
log10ws	-0.55		Crippen Method
logp	0.465		Crippen Method
mcvol	117.710	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C26608582&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/23-343-5/1-Azabicyclo-2-2-2-octane-4-methanol.pdf>

Generated by Cheméo on 2024-04-26 22:12:07.835454792 +0000 UTC m=+16458776.756032107.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.