1-Azabicyclo[2.2.2]octane-4-ol acetate(ester)

Other names: 4-Acetoxy-1-azabicyclo[2.2.2]octane
Inchi: InChI=1S/C9H15NO2/c1-8(11)12-9-2-5-10(6-3-9)7-4-9/h2-7H2,1H3
InchiKey: XTKZIFBRSPNTJD-UHFFFAOYSA-N
Formula: C9H15NO2
SMILES: CC(=O)OC12CCN(CC1)CC2
Mol. weight [g/mol]: 169.22
CAS: 26458-76-4

Physical Properties

Property code	Value	Unit	Source
ie	8.42 ± 0.01	eV	NIST Webbook
log10ws	-0.92		Crippen Method
logp	0.788		Crippen Method
mcvol	133.370	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=C26458764&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

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