8-Azabicyclo[3.2.1]octan-3-ol,8-methyl-methylcarb

Inchi: InChI=1S/C10H18N2O2/c1-11-10(13)14-9-5-7-3-4-8(6-9)12(7)2/h7-9H,3-6H2,1-2H3,(H,1
InchiKey: UJPUERKEXKHUAG-UHFFFAOYSA-N
Formula: C10H18N2O2
SMILES: CNC(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 198.26
CAS: 67139-52-0

Physical Properties

Property code	Value	Unit	Source
ie	8.20 ± 0.15	eV	NIST Webbook
log10ws	-1.73		Crippen Method
logp	0.968		Crippen Method
mcvol	157.440	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=C67139520&Units=SI

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.