7-Azabicyclo[2.2.1]heptane-7-carboxylic acid, methyl ester

Inchi: InChI=1S/C8H13NO2/c1-11-8(10)9-6-2-3-7(9)5-4-6/h6-7H,2-5H2,1H3
InchiKey: VYMRJKGRCMURSL-UHFFFAOYSA-N
Formula: C8H13NO2
SMILES: COC(=O)N1C2CCC1CC2
Mol. weight [g/mol]: 155.19
CAS: 131179-08-3

Physical Properties

Property code	Value	Unit	Source
ie	8.30	eV	NIST Webbook
ie	8.93	eV	NIST Webbook
log10ws	-1.59		Crippen Method
logp	1.380		Crippen Method
mcvol	119.280	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=C131179083&Units=SI

Legend

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