5,6-Dihydro-7,9-dimethoxy-7H-pyrrolizine

Inchi: InChI=1S/C10H17NO2/c1-12-7-8-3-5-11-6-4-9(13-2)10(8)11/h3,9-10H,4-7H2,1-2H3/t9-,1
InchiKey: NTHXXXBCILAZIH-RGURZIINSA-N
Formula: C10H17NO2
SMILES: COCC1=CCN2CCC(OC)C12
Mol. weight [g/mol]: 183.25

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.62		Crippen Method
logp	0.662		Crippen Method
mcvol	147.460	ml/mol	McGowan Method
rinpol	1413.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1415.00		NIST Webbook
rinpol	1413.00		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=R240492&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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