(+)-1-Hydroxymethyl- pyrrolizidine butanoic acid ester

Inchi: InChI=1S/C12H21NO2/c1-2-4-12(14)15-9-10-6-8-13-7-3-5-11(10)13/h10-11H,2-9H2,1H3

InchiKey: LSWFXZFXZVYUMB-UHFFFAOYSA-N

Formula: C12H21NO2

SMILES: CCCC(=O)OCC1CCN2CCCC12

Mol. weight [g/mol]: 211.30

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.94		Crippen Method
logp	1.814		Crippen Method
mcvol	175.640	ml/mol	McGowan Method
rinpol	1667.00		NIST Webbook
rinpol	1710.00		NIST Webbook
rinpol	1667.00		NIST Webbook

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=R335218&Units=SI

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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