

[(7R)-7-Hydroxy-5,6,7,8-tetrahydro-3H-pyrrolizin-1-yl]-methyl-hexanoate

InChI: InChI=1S/C14H23NO3/c1-2-3-4-5-13(17)18-10-11-6-8-15-9-7-12(16)14(11)15/h6,12,14,17
InChIKey: QOICZOKWVHLXDD-NBFOIZRFSA-N
Formula: C14H23NO3
SMILES: CCCCCC(=O)OCC1=CCN2CCC(O)C12
Mol. weight [g/mol]: 253.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.25		Crippen Method
logp	1.485		Crippen Method
mcvol	205.390	ml/mol	McGowan Method
rinpol	1885.00		NIST Webbook
rinpol	1885.00		NIST Webbook

Sources

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R577952&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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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