

# [(1R)-7-(Hydroxymethyl)-2,3,5,8-tetrahydro-1H-pyrrolizin-1-yl]hexanoate

InChI: InChI=1S/C15H25NO3/c1-2-3-4-5-14(18)19-11-13-7-9-16-8-6-12(10-17)15(13)16/h6,13,14,15,16,17,18,19  
InChIKey: LFJHJPZPFBAHID-CFMCSPISA-N  
Formula: C15H25NO3  
SMILES: CCCCCC(=O)OCC1CCN2CC=C(CO)C12  
Mol. weight [g/mol]: 267.36

## Physical Properties

Property code	Value	Unit	Source
log10ws	-2.31		Crippen Method
logp	1.733		Crippen Method
mcvol	219.480	ml/mol	McGowan Method
rinpol	1870.00		NIST Webbook
rinpol	1870.00		NIST Webbook

## Sources

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.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=R577794&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

Latest version available from:

<https://www.cheméo.com/cid/20-274-5/1R-7-Hydroxymethyl-2-3-5-8-tetrahydro-1H-pyrrolizin-1-yl-hexanoate.pdf>

Generated by Cheméo on 2024-04-26 09:22:40.511504734 +0000 UTC m=+16412609.432082049.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.