

# 3-Hexanoyloxytropane

**Inchi:** InChI=1S/C14H25NO2/c1-3-4-5-6-14(16)17-13-9-11-7-8-12(10-13)15(11)2/h11-13H,3-10H  
**InchiKey:** GVIXUEFDNNKUEZ-FUNVUKJBSA-N  
**Formula:** C14H25NO2  
**SMILES:** CCCCCC(=O)OC1CC2CCC(C1)N2C  
**Mol. weight [g/mol]:** 239.35

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.24		Crippen Method
logp	2.735		Crippen Method
mcvol	203.820	ml/mol	McGowan Method
rinpol	1755.00		NIST Webbook
rinpol	1755.00		NIST Webbook

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R509805&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**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>

## 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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