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,3-10
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

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=R509805&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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