6-(Hydroxybutyroxy)-3-pentanoyloxytropane

Inchi: InChI=1S/C17H29NO5/c1-4-6-7-16(20)22-12-8-11-9-15(13(10-12)18(11)3)23-17(21)14(1
InchiKey: YDGSNTGTXDVICB-AAGZUDIBSA-N
Formula: C17H29NO5
SMILES: CCCCC(=O)OC1CC2CC(OC(=O)C(O)CC)C(C1)N2C
Mol. weight [g/mol]: 327.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.85		Crippen Method
logp	1.638		Crippen Method
mcvol	259.400	ml/mol	McGowan Method
rinpol	2150.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R509969&Units=SI
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

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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