3-Phenylacetoxy-6-hydroxytropane

Inchi: InChI=1S/C16H21NO3/c1-17-12-8-13(10-14(17)15(18)9-12)20-16(19)7-11-5-3-2-4-6-11/l
InchiKey: NHJIGOBHFARUPD-FGZQJIAISA-N
Formula: C16H21NO3
SMILES: CN1C2CC(OC(=O)Cc3ccccc3)CC1C(O)C2
Mol. weight [g/mol]: 275.34

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.56		Crippen Method
logp	1.368		Crippen Method
mcvol	214.110	ml/mol	McGowan Method
rinpol	2049.00		NIST Webbook
rinpol	2049.00		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=R421646&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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