

Tropanyl (2-acetoxy-3-(para-hydroxyphenyl)propanoate)

Inchi: InChI=1S/C19H25NO5/c1-12(21)24-18(9-13-3-7-16(22)8-4-13)19(23)25-17-10-14-5-6-15
InchiKey: LDWBSZBICDWOCG-UHFFFAOYSA-N
Formula: C19H25NO5
SMILES: CC(=O)OC(Cc1ccc(O)cc1)C(=O)OC1CC2CCC(C1)N2C
Mol. weight [g/mol]: 347.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	2.035		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
rinpol	2975.60		NIST Webbook
rinpol	2975.60		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: 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=U415027&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

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