

3-Tropoyloxy-6-acetoxytropane

Inchi: InChI=1S/C19H25NO5/c1-12(22)24-18-9-14-8-15(10-17(18)20(14)2)25-19(23)16(11-21)
InchiKey: HMSYCWNYGYVPME-FEPQMPSTSA-N
Formula: C19H25NO5
SMILES: CC(=O)OC1CC2CC(OC(=O)C(CO)c3ccccc3)CC1N2C
Mol. weight [g/mol]: 347.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.64		Crippen Method
logp	1.473		Crippen Method
mcvol	263.820	ml/mol	McGowan Method
rinpol	2367.00		NIST Webbook
rinpol	2367.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R421715&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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