

Benzoyltropeine

Other names: 3«alpha»-Benzoyloxytropane
Inchi: InChI=1S/C15H19NO2/c1-16-12-7-8-13(16)10-14(9-12)18-15(17)11-5-3-2-4-6-11/h2-6,12-14
InchiKey: XQJMXPAEFMWDOZ-WDNDVIMCSA-N
Formula: C15H19NO2
SMILES: CN1C2CCC1CC(OC(=O)c1ccccc1)C2
Mol. weight [g/mol]: 245.32

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.34		Crippen Method
logp	2.469		Crippen Method
mcvol	194.150	ml/mol	McGowan Method
rinpol	1968.00		NIST Webbook
rinpol	1930.00		NIST Webbook
rinpol	1907.00		NIST Webbook
rinpol	1907.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R152904&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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