3«alpha»-Phenylacetoxytropane

Inchi: InChI=1S/C16H21NO2/c1-17-13-7-8-14(17)11-15(10-13)19-16(18)9-12-5-3-2-4-6-12/h2-
InchiKey: DCINQANYMBYYCH-UHFFFAOYSA-N
Formula: C16H21NO2
SMILES: CN1C2CCC1CC(OC(=O)Cc1ccccc1)C2
Mol. weight [g/mol]: 259.34
CAS: 1690-22-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.18		Crippen Method
logp	2.398		Crippen Method
mcvol	208.240	ml/mol	McGowan Method
rinpol	2014.40		NIST Webbook
rinpol	2014.40		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C1690228&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices