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

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
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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