

1-Methyl-3-piperidyl cyclopentylphenylglycolate

Inchi: InChI=1S/C19H27NO3/c1-20-13-7-12-17(14-20)23-18(21)19(22,16-10-5-6-11-16)15-8-3
InchiKey: SEWHBJAHHOCKER-UHFFFAOYSA-N
Formula: C19H27NO3
SMILES: CN1CCCC(OC(=O)C(O)(c2ccccc2)C2CCCC2)C1
Mol. weight [g/mol]: 317.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.702		Crippen Method
mcvol	256.380	ml/mol	McGowan Method
rinpol	2280.00		NIST Webbook
rinpol	2374.00		NIST Webbook
rinpol	2280.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.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=U289597&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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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<https://www.chemeo.com/cid/22-762-1/1-Methyl-3-piperidyl-cyclopentylphenylglycolate.pdf>

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