Mandelic acid, «alpha»-cyclopentyl-, 1-methyl-4-piperidyl ester

Other names: Benzeneacetic acid, «alpha»-cyclopentyl-«alpha»-hydroxy-, 1-methyl-4-piperidinyl ester
EA 3443
N-Methyl-4-piperidyl cyclopentylphenylglycolate
1-Methyl-4-piperidyl cyclopentylphenylglycolate
Benzeneacetic acid, alpha-cyclopentyl-alpha-hydroxy-, 1-methyl-4-piperidinyl ester

Inchi: InChI=1S/C19H27NO3/c1-20-13-11-17(12-14-20)23-18(21)19(22,16-9-5-6-10-16)15-7-3-

InchiKey: DZFJGXMHIMAYMW-UHFFFAOYSA-N

Formula: C19H27NO3

SMILES: CN1CCC(OC(=O)C(O)(c2ccccc2)C2CCCC2)CC1

Mol. weight [g/mol]: 317.42

CAS: 37830-21-0

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	2310.00		NIST Webbook

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C37830210&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices