1-Methyl-4-piperidyl cyclopentylphenylglycolate

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]: 317.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.06		Cheméo Relay (1.0)
logp	2.702		Crippen Method
mcvol	256.380	ml/mol	McGowan Method
rinpol	2310.00		NIST Webbook
tf	389.13	K	Cheméo Relay (1.0)

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

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
tf:	Normal melting (fusion) point