

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

Other names:	Benzeneacetic acid, «alpha»-cyclopentyl-«alpha»-hydroxy-, 1-methyl-4-piperidiny ester EA 3443 N-Methyl-4-piperidyl cyclopentylphenylglycolate 1-Methyl-4-piperidyl cyclopentylphenylglycolate Benzeneacetic acid, alpha-cyclopentyl-alpha-hydroxy-, 1-methyl-4-piperidiny 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
rinsol	2310.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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