

# Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 1-methyl-3-piperidiny ester

Other names:

Benzilic acid, 1-methyl-3-piperidyl ester  
JB 336

N-Methyl-3-piperidyl benzilate

1-Methyl-3-piperidyl benzilate

1-Methyl-3-piperidyl benzylate

Inchi:

InChI=1S/C20H23NO3/c1-21-14-8-13-18(15-21)24-19(22)20(23,16-9-4-2-5-10-16)17-11-

InchiKey:

ZBEILXWHVSVDBN-UHFFFAOYSA-N

Formula:

C20H23NO3

SMILES:

CN1CCCC(OC(=O)C(O)(c2ccccc2)c2ccccc2)C1

Mol. weight [g/mol]:

325.40

CAS:

3321-80-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.560		Crippen Method
mcvol	257.570	ml/mol	McGowan Method

## Sources

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](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=C3321800&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

## Legend

log10ws:

Log10 of Water solubility in mol/l

logp:

Octanol/Water partition coefficient

mcvol:

McGowan's characteristic volume

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