

Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 1-methyl-4-piperidyl ester

Other names:

4-NMPB

1-Methyl-4-piperidyl benzilate

«alpha»-Hydroxy-diphenylacetic acid, 1-methyl -4-piperidiny ester

1-Methyl-4-piperidyl benzylate

Enpiperate

NSC 172167

1-methyl-4-piperidyl diphenylglycolate

Inchi:

InChI=1S/C20H23NO3/c1-21-14-12-18(13-15-21)24-19(22)20(23,16-8-4-2-5-9-16)17-10-

InchiKey:

UGYPGJCVNPPUPE-UHFFFAOYSA-N

Formula:

C20H23NO3

SMILES:

CN1CCC(OC(=O)C(O)(c2ccccc2)c2ccccc2)CC1

Mol. weight [g/mol]:

325.40

CAS:

3608-67-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.37		Crippen Method
logp	2.560		Crippen Method
mcvol	257.570	ml/mol	McGowan Method
rmpol	2431.00		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=C3608671&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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