

.alpha.-hydroxy-diphenylacetic acid, 1-methyl-4-piperidiny 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]: 325.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.96		Cheméo Relay (1.0)
logp	2.560		Crippen Method
mcvol	257.570	ml/mol	McGowan Method
tf	385.49	K	Cheméo Relay (1.0)

Sources

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=C3608671&Units=SI>

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tf:	Normal melting (fusion) point

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