Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 1-methyl-3-piperidinyl 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
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/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume