3-Quinuclidinyl benzilate

Other names:	BZ
	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 1-azabicyclo(2.2.2)oct-3-yl ester
	QNB
	RO 2-3308
	Benzilic acid, 3-quinuclidinyl ester
	1-Azabicyclo(2.2.2)octan-3-ol, benzilate
	3-Chinuclidylbenzilate
	CS 4030
	EA 2277
	3-Quinuclidinol benzilate
	3-Quinuclidinol, benzilate (ester)
	«beta»-Quinuclidinyl benzilate
	3-Hydroxyquinuclidine benzilate
	3-Oxyquinuclidine benzilate
	3-Quinuclidyl benzilate
	Agent BZ
	NSC 173698
Inchi:	InChI=1S/C21H23NO3/c23-20(25-19-15-22-13-11-16(19)12-14-22)21(24,17-7-3-1-4-8-17
InchiKey:	HGMITUYOCPPQLE-UHFFFAOYSA-N
Formula:	C21H23NO3
SMILES:	O=C(OC1CN2CCC1CC2)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	337.41
CAS:	6581-06-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.45		Crippen Method
logp	2.560		Crippen Method
mcvol	260.800	ml/mol	McGowan Method
rinpol	2628.00		NIST Webbook
rinpol	2628.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C6581062&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