2-Piperidin-1-ylethyl hydroxy(diphenyl)acetate

Other names:	Benzilic acid, 2-piperidinoethyl ester
	Benzeneacetic acid, «alpha»-hydroxy-«alpha»-phenyl-, 2-(1-piperidinyl)ethyl ester
	1-Piperidineethanol benzilate
	2-(1-Piperidino)ethyl benzilate
	«beta»-Piperidylethyl benzilate
	Pipethanate
	«alpha»-Hydroxy-«alpha»-phenylbenzeneacetic acid 2-(1-piperidinyl)ethyl ester
Inchi:	InChI=1S/C21H25NO3/c23-20(25-17-16-22-14-8-3-9-15-22)21(24,18-10-4-1-5-11-18)19-
InchiKey:	RZWPJFMNFATBEG-UHFFFAOYSA-N
Formula:	C21H25NO3
SMILES:	O=C(OCCN1CCCCC1)C(O)(c1ccccc1)c1ccccc1
Mol. weight [g/mol]:	339.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.57		Cheméo Relay (1.0)
logp	2.952		Crippen Method
mcvol	271.660	ml/mol	McGowan Method
rinpol	2464.00		NIST Webbook
rinpol	2475.00		NIST Webbook
tb	670.27	K	Cheméo Relay (1.0)
tf	357.02	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):	
Cheméo Relay (1.0, beta):	
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C4546398&Units=SI
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point