Piperidolate

Other names:	Benzeneacetic acid, «alpha»-phenyl-, 1-ethyl-3-piperidinyl ester
	Acetic acid, diphenyl-, 1-ethyl-3-piperidyl ester
	Dactil
	Diphenylacetic acid, 1-ethyl-3-piperidyl ester
	JB 305
	N-Ethyl-3-Piperidyl diphenylacetate
	1-Ethyl-3-piperidyl diphenylacetate
	AN 1087
	3-Piperidinol, 1-ethyl-, diphenylacetate
	1087 A.N.
	3-Piperidinol, 1-ethyl-, diphenylacetate (ester)
Inchi:	InChI=1S/C21H25NO2/c1-2-22-15-9-14-19(16-22)24-21(23)20(17-10-5-3-6-11-17)18-12-
InchiKey:	KTHVBAZBLKXIHZ-UHFFFAOYSA-N
Formula:	C21H25NO2
SMILES:	CCN1CCCC(OC(=O)C(c2ccccc2)c2ccccc2)C1
Mol. weight [g/mol]:	323.43
CAS:	82-98-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.32		Crippen Method
logp	3.846		Crippen Method
mcvol	265.790	ml/mol	McGowan Method
rinpol	2316.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2347.00		NIST Webbook
rinpol	2318.00		NIST Webbook
rinpol	2360.00		NIST Webbook
rinpol	2316.00		NIST Webbook
rinpol	2347.00		NIST Webbook
rinpol	2343.00		NIST Webbook
rinpol	2343.00		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=C82984&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