Benzquinamide

Other names:	2H-Benzo[a]quinolizine-3-carboxamide, 2-(acetyloxy)-N,N-diethyl-1,3,4,6,7,11b-hexahydro-9,10-dimethoxy-
	N,N-Diethyl-1,3,4,6,7,11b-hexahydro-2-hydroxy-9,10-dimethoxy-2H-benzo[a]quinolizine-3
	Benzchinamide
	acetate (ester)
	2-(Acetoxy)-N,N-diethyl-1,3,4,6,7,11b-hexahydro-9,10-diemethoxy-2H-benzo[a]quinolizin
	BZQ
	Emete-Con
	Emeticon
	NSC-64375
	P-2647
	Promecon
	2H-Benzo(a)quinolizine-3-carboxamide, N,N-diethyl-1,3,4,6,7,11b-hexahydro-2-hydroxy-9,10-dimethoxy-, acetate (ester)
	2-Hydroxy-3-diethylcarbamyl-9,10-dimethoxy-1,2,3,4,6,7-hexahydro-11bH-benzoquinolizi
	Benzoquinamide
	acetate
	Benzochinamide
Inchi:	InChI=1S/C22H32N2O5/c1-6-23(7-2)22(26)17-13-24-9-8-15-10-20(27-4)21(28-5)11-16(1
InchiKey:	JSZILQVIPPROJI-UHFFFAOYSA-N
Formula:	C22H32N2O5
SMILES:	CCN(CC)C(=O)C1CN2CCc3cc(OC)c(OC)cc3C2CC1OC(C)=O
Mol. weight [g/mol]:	404.50
CAS:	63-12-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.40		Crippen Method
logp	2.423		Crippen Method
mcvol	316.070	ml/mol	McGowan Method
rinpol	2980.00		NIST Webbook
rinpol	2980.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C63127&Units=SI
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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices