Benzquinamide M (N-des-Et), acetylated

Inchi:	InChI=1S/C22H30N2O6/c1-6-24(13(2)25)22(27)17-12-23-8-7-15-9-20(28-4)21(29-5)10-1
InchiKey:	KYXZHWVPMPALKB-UHFFFAOYSA-N
Formula:	C22H30N2O6
SMILES:	CCN(C(C)=O)C(=O)C1CN2CCc3cc(OC)c(OC)cc3C2CC1OC(C)=O
Mol. weight [g/mol]:	418.48

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.17		Crippen Method
logp	1.950		Crippen Method
mcvol	317.640	ml/mol	McGowan Method
rinpol	2960.00		NIST Webbook
rinpol	2960.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R120497&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

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