

Benzquinamide M (O-des-Et), acetylated

Inchi:	InChI=1S/C23H32N2O6/c1-6-24(7-2)23(28)18-13-25-9-8-16-10-22(31-15(4)27)21(29-5)1
InchiKey:	WQUOYBGLIUNALZ-UHFFFAOYSA-N
Formula:	C23H32N2O6
SMILES:	CCN(CC)C(=O)C1CN2CCc3cc(OC(C)=O)c(OC)cc3C2CC1OC(C)=O
Mol. weight [g/mol]:	432.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.340		Crippen Method
mcvol	331.730	ml/mol	McGowan Method
rinpola	2990.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=R120506&Units=SI

Legend

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

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<https://www.chemeo.com/cid/65-043-2/Benzquinamide-M-O-des-Et-acetylated.pdf>

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