

Tetrabenazine M (bis-desmethyl-HO-), diacetylated

Inchi:	InChI=1S/C21H27NO5/c1-12(2)7-16-11-22-6-5-15-8-20(26-13(3)23)21(27-14(4)24)9-17(
InchiKey:	UTUCIZUVPRMZBM-UHFFFAOYSA-N
Formula:	C21H27NO5
SMILES:	CC(=O)Oc1cc2c(cc1OC(C)=O)C1CC(=O)C(CC(C)C)CN1CC2
Mol. weight [g/mol]:	373.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.25		Crippen Method
logp	3.071		Crippen Method
mcvol	287.700	ml/mol	McGowan Method
rinpole	2666.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R310660&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.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
rinpole:	Non-polar retention indices

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