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
rinpol	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/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