Tetrabenazine M (desmethyl-HO-), monoacetylated

Inchi: InChI=1S/C20H27NO5/c1-11(2)7-13-10-21-6-5-14-15(16(21)9-17(13)23)8-18(26-12(3)22
InchiKey: KEWYAANPLZTFIO-UHFFFAOYSA-N
Formula: C20H27NO5
SMILES: COc1c(OC(C)=O)cc2c(c1O)CCN1CC(CC(C)C)C(=O)CC21
Mol. weight [g/mol]: 361.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.60		Crippen Method
logp	2.860		Crippen Method
mcvol	277.910	ml/mol	McGowan Method
rinpol	2584.00		NIST Webbook
rinpol	2584.00		NIST Webbook

Sources

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
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R310675&Units=SI

Legend

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

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.