Tetrabenazine M (bis-desmethyl-), monoacetylated

Inchi: InChI=1S/C19H25NO4/c1-11(2)6-14-10-20-5-4-13-7-18(23)19(24-12(3)21)8-15(13)16(20

InchiKey: SNIFFGCVFZKOJF-UHFFFAOYSA-N

Formula: C19H25NO4

SMILES: CC(=O)Oc1cc2c(cc1O)CCN1CC(CC(C)C)C(=O)CC21

Mol. weight [g/mol]: 331.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.48		Crippen Method
logp	2.852		Crippen Method
mcvol	257.950	ml/mol	McGowan Method
rinpol	2510.00		NIST Webbook
rinpol	2510.00		NIST Webbook

Sources

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=R310655&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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.