Acetylsenecivernine

Inchi: InChI=1S/C20H27NO6/c1-11-12(2)18(23)26-16-7-9-21-8-6-15(17(16)21)10-25-19(24)20(
InchiKey: NYUTVFRDPMUSRA-HVFAAYSOSA-N
Formula: C20H27NO6
SMILES: C=C1C(=O)OC2CCN3CC=C(COC(=O)C(C)(OC(C)=O)C(C)C1C)C23
Mol. weight [g/mol]: 377.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	1.620		Crippen Method
mcvol	283.780	ml/mol	McGowan Method
rinpol	2450.00		NIST Webbook
rinpol	2450.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R405302&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

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