Jaconine

Inchi: InChI=1S/C18H26ClNO6/c1-10-8-18(24,11(2)19)16(22)26-13-5-7-20-6-4-12(14(13)20)9-
InchiKey: CKPJPJSVQMEGBC-UHFFFAOYSA-N
Formula: C18H26ClNO6
SMILES: CC1CC(O)(C(C)Cl)C(=O)OC2CCN3CC=C(COC(=O)C1(C)O)C23
Mol. weight [g/mol]: 387.86
CAS: 480-75-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.19		Crippen Method
logp	0.605		Crippen Method
mcvol	276.440	ml/mol	McGowan Method
rinpol	2548.00		NIST Webbook
rinpol	2520.00		NIST Webbook
rinpol	2527.00		NIST Webbook
rinpol	2573.00		NIST Webbook
rinpol	2584.00		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=C480751&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