Adonifoline

Inchi: InChI=1S/C18H23NO7/c1-10-18(22)8-17(9-24-10)16(2,26-17)14(20)23-7-11-3-5-19-6-4-1
InchiKey: MYOFCWPLRKBPJD-AQYQBICXSA-N
Formula: C18H23NO7
SMILES: CC1OCC23CC1(O)C(=O)OC1CCN4CC=C(COC(=O)C2(C)O3)C14
Mol. weight [g/mol]: 365.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.09		Crippen Method
logp	-0.463		Crippen Method
mcvol	248.350	ml/mol	McGowan Method
rinpol	2530.00		NIST Webbook
rinpol	2545.00		NIST Webbook
rinpol	2530.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R177869&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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