cyclomegistine

Inchi: InChI=1S/C18H21NO7/c1-19-11-9-7-6-8-10(11)13(20)12-14(19)18(26-5,16(22)24-3)17(1
InchiKey: KNMICIOSHLUGSP-VQHUDLGKSA-N
Formula: C18H21NO7
SMILES: COC(=O)C1(OC)C2C(=O)c3ccccc3N(C)C2C1(OC)C(=O)OC
Mol. weight [g/mol]: 363.36

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.17		Crippen Method
logp	0.434		Crippen Method
mcvol	257.170	ml/mol	McGowan Method
rinpol	2736.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R285693&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