Crosemperine ethyl analogue

Inchi: InChI=1S/C18H27NO6/c1-5-13-11(2)18(3,23)17(22)24-10-12-6-8-19(4)9-7-14(15(12)20)
InchiKey: JSRISOTXWALVLP-KKKSXTILSA-N
Formula: C18H27NO6
SMILES: CCC1C(=O)OC2CCN(C)CC=C(COC(=O)C(C)(O)C1C)C2=O
Mol. weight [g/mol]: 353.41

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.58		Crippen Method
logp	0.699		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2487.00		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=R590262&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