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
logp	0.699		Crippen Method
mcvol	270.760	ml/mol	McGowan Method
rinpol	2487.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R590262&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

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https://www.chemeo.com/cid/58-935-0/Crosemperine-ethyl-analogue.pdf
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