Crosemperine stereoisomer

Inchi: InChI=1S/C19H29NO6/c1-11(2)15-12(3)19(4,24)18(23)25-10-13-6-8-20(5)9-7-14(16(13)2
InchiKey: MODJNYOZJNBECF-RFKTUILYSA-N
Formula: C19H29NO6
SMILES: CC(C)C1C(=O)O[C@@H]2CCN(C)C/C=C(/COC(=O)C(C)(O)C1C)C2=O
Mol. weight [g/mol]: 367.44

Physical Properties

Property code	Value	Unit	Source
logp	0.945		Crippen Method
mcvol	284.850	ml/mol	McGowan Method
rinpol	2615.00		NIST Webbook

Sources

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=R590277&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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