(Z)-Cnidimine

Inchi: InChI=1S/C21H22O7/c1-6-11(2)20(24)27-18-16-14(25-19(18)21(4,5)28-12(3)22)9-7-13-8
InchiKey: FFCDTHIJWHJUQJ-WDZFZDKYSA-N
Formula: C21H22O7
SMILES: CC=C(C)C(=O)OC1c2c(ccc3ccc(=O)oc23)OC1C(C)(C)OC(C)=O
Mol. weight [g/mol]: 386.40
CAS: 15591-75-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.28		Crippen Method
logp	3.446		Crippen Method
mcvol	280.860	ml/mol	McGowan Method
rinpol	2822.40		NIST Webbook
rinpol	2822.40		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C15591750&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