

DILTIAZEM, M(DESAMINO-HO-), AC

Inchi: InChI=1S/C22H23NO6S/c1-14(24)28-13-12-23-18-6-4-5-7-19(18)30-21(20(22(23)26)29-
InchiKey: YLUJWLVMYSNGT-RTWAWAEBSA-N
Formula: C22H23NO6S
SMILES: COc1ccc(C2Sc3ccccc3N(CCOC(C)=O)C(=O)C2OC(C)=O)cc1
Mol. weight [g/mol]: 429.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.370		Crippen Method
mcvol	311.110	ml/mol	McGowan Method
rinpola	3060.00		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=R255048&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
rinpola: Non-polar retention indices

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