DILTIAZEM, M(ODESMETHYL-), AC

Inchi: InChI=1S/C23H26N2O5S/c1-15(26)29-18-11-9-17(10-12-18)22-21(30-16(2)27)23(28)25(

InchiKey: XNHIWNXIIJPWLD-FCHUYYIVSA-N

Formula: C23H26N2O5S

SMILES: CC(=O)Oc1ccc(C2Sc3ccccc3N(CCN(C)C)C(=O)C2OC(C)=O)cc1

Mol. weight [g/mol]:   442.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.24		Crippen Method
logp	3.285		Crippen Method
mcvol	329.310	ml/mol	McGowan Method
rinpol	3080.00		NIST Webbook
rinpol	3080.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315952&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

rinpol: Non-polar retention indices

Latest version available from:

https://www.chemeo.com/cid/47-551-8/DILTIAZEM-M-ODESMETHYL-AC.pdf

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