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

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R315952&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.