DILTIAZEM, M(O-DESMETHYL-DESAMINO-HO-), AC

Inchi: InChI=1S/C23H23NO7S/c1-14(25)29-13-12-24-19-6-4-5-7-20(19)32-22(21(23(24)28)31-
InchiKey: BZRJHJFJQUZPGT-YADHBBJMSA-N
Formula: C23H23NO7S
SMILES: CC(=O)OCCN1C(=O)C(OC(C)=O)C(c2ccc(OC(C)=O)cc2)Sc2ccccc21
Mol. weight [g/mol]: 457.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.53		Crippen Method
logp	3.287		Crippen Method
mcvol	326.770	ml/mol	McGowan Method
rinpol	3170.00		NIST Webbook
rinpol	3170.00		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=R315967&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
rinpol: Non-polar retention indices

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