Diltiazem

Other names:	Dilacor XR
	Cardizem
	1,5-Benzothiazepin-4(5H)-one, 3-(acetyloxy)-5-[2-(dimethylamino)ethyl]-2,3-dihydro-2-(4-methoxyphenyl)-, (2S-cis)-
	(+)-5-[2-(Dimethylamino)ethyl]-cis-2,3-dihydro-3-hydroxy-2-(p-methoxyphenyl)-1,5-benzot
	Tiazac acetate (ester)
Inchi:	InChI=1S/C22H26N2O4S/c1-15(25)28-20-21(16-9-11-17(27-4)12-10-16)29-19-8-6-5-7-18
InchiKey:	HSUGRBWQSSZJOP-UHFFFAOYSA-N
Formula:	C22H26N2O4S
SMILES:	COc1ccc(C2Sc3ccccc3N(CCN(C)C)C(=O)C2OC(C)=O)cc1
Mol. weight [g/mol]:	414.52
CAS:	42399-41-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.04		Crippen Method
logp	3.369		Crippen Method
mcvol	313.650	ml/mol	McGowan Method
rinpol	2960.00		NIST Webbook
rinpol	2927.00		NIST Webbook
rinpol	2960.00		NIST Webbook
rinpol	2927.00		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=C42399417&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

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