Valsartan 2Me

Inchi: InChI=1S/C26H33N5O3/c1-6-7-12-23(32)31(24(18(2)3)26(33)34-5)17-19-13-15-20(16-14
InchiKey: WGMNSNVXRKWQKB-XMMPIXPASA-N
Formula: C26H33N5O3
SMILES: CCCCC(=O)N(Cc1ccc(-c2ccccc2-c2nnn(C)n2)cc1)C(C(=O)OC)C(C)C
Mol. weight [g/mol]: 463.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.82		Crippen Method
logp	4.260		Crippen Method
mcvol	369.130	ml/mol	McGowan Method
rinpol	3420.00		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=R550046&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