Mepindolol, acetylated

Inchi: InChI=1S/C21H28N2O4/c1-14(2)23(16(4)25)13-19(27-17(5)26)10-9-18-7-6-8-21-20(18)1
InchiKey: JOQPPRNDHFGXLN-UHFFFAOYSA-N
Formula: C21H28N2O4
SMILES: CC(=O)OC(CCc1cccc2c1ccn2C(C)=O)CN(C(C)=O)C(C)C
Mol. weight [g/mol]: 372.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.40		Crippen Method
logp	3.423		Crippen Method
mcvol	298.370	ml/mol	McGowan Method
rinpol	2390.00		NIST Webbook
rinpol	2390.00		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R582682&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.