

Carazolol, acetylated

Inchi: InChI=1S/C25H30N2O5/c1-16(2)26(17(3)28)14-13-20(32-19(5)30)15-31-24-12-8-11-23-2
InchiKey: CGGFBGDEBZRJLJ-UHFFFAOYSA-N
Formula: C25H30N2O5
SMILES: CC(=O)OC(CCN(C(C)=O)C(C)C)COc1cccc2c1c1cccc1n2C(C)=O
Mol. weight [g/mol]: 438.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.94		Crippen Method
logp	4.412		Crippen Method
mcvol	341.140	ml/mol	McGowan Method
rinpol	2810.00		NIST Webbook
rinpol	2810.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R582573&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>

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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