

Cinnarizine M (carbinol), acetylated

Inchi: InChI=1S/C28H30N2O2/c1-24(31)32-28(26-15-7-3-8-16-26,27-17-9-4-10-18-27)30-22-20
InchiKey: JBYBHZSAOUIVHG-KAMYIIQDSA-N
Formula: C28H30N2O2
SMILES: CC(=O)OC(c1ccccc1)(c1ccccc1)N1CCN(CC=Cc2ccccc2)CC1
Mol. weight [g/mol]: 426.55

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.54 | | Crippen Method |
| logp | 4.782 | | Crippen Method |
| mcvol | 346.340 | ml/mol | McGowan Method |
| rinpole | 1700.00 | | 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=R536179&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpole: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/27-618-6/Cinnarizine-M-carbinol-acetylated.pdf>

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