

carpipramine

Inchi: InChI=1S/C28H38N4O/c29-27(33)28(31-18-6-1-7-19-31)15-21-30(22-16-28)17-8-20-32-2
InchiKey: NWPJLRSCSQHPJV-UHFFFAOYSA-N
Formula: C28H38N4O
SMILES: NC(=O)C1(N2CCCCC2)CCN(CCCN2c3ccccc3CCc3ccccc32)CC1
Mol. weight [g/mol]: 446.63
CAS: 5942-95-0

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -5.53 | | Crippen Method |
| logp | 4.119 | | Crippen Method |
| mcvol | 366.770 | ml/mol | McGowan Method |
| rinpola | 3722.00 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C5942950&Units=SI>
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>

Legend

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

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<https://www.chemeo.com/cid/39-218-7/carpipramine.pdf>

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