

3'-cis-cinnamoylindicine

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|-----------------------------|--|
| Inchi: | InChI=1S/C24H31NO6/c1-16(2)24(29,17(3)31-21(27)10-9-18-7-5-4-6-8-18)23(28)30-15- |
| InchiKey: | PJJDYGUZICJPQG-PFWUHNAQSA-N |
| Formula: | C24H31NO6 |
| SMILES: | CC(C)C(O)(C(=O)OCC1=CCN2CCC(O)C12)C(C)OC(=O)C=Cc1ccccc1 |
| Mol. weight [g/mol]: | 429.51 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -3.66 | | Crippen Method |
| logp | 1.937 | | Crippen Method |
| mcvol | 331.540 | ml/mol | McGowan Method |
| rinpola | 2925.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R516497&Units=SI |

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/66-254-7/3-cis-cinnamoylindicine.pdf>

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