13-Trans-cinnamoyloxylupanine

Inchi: InChI=1S/C24H30N2O3/c27-23-8-4-7-21-18-13-19(16-26(21)23)22-14-20(11-12-25(22)1
InchiKey: PUFYZCKVLOYPHL-KVXFRRANSA-N
Formula: C24H30N2O3
SMILES: O=C(C=Cc1ccccc1)OC1CCN2CC3CC(CN4C(=O)CCCC34)C2C1
Mol. weight [g/mol]: 394.51

Physical Properties

Property code	Value	Unit	Source
logp	3.107		Crippen Method
mcvol	306.490	ml/mol	McGowan Method
rinpol	3390.00		NIST Webbook

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R308484&Units=SI
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):

Legend

logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
rinpol: Non-polar retention indices

Latest version available from:
https://www.chemeo.com/cid/13-094-3/13-Trans-cinnamoyloxylupanine.pdf
Generated by Cheméo on 2026-07-21 15:08:31.219081239 +0000 UTC m=+157607.060966641.
Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.