

(E)-11-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)

Inchi: InChI=1S/C23H33NO3/c25-23(24-16-10-7-11-17-24)13-9-6-4-2-1-3-5-8-12-20-14-15-21-1
InchiKey: RYLSVPVFBOMQMG-XYOKQWHBSA-N
Formula: C23H33NO3
SMILES: O=C(CCCCCCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 371.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.61		Crippen Method
logp	5.562		Crippen Method
mcvol	308.440	ml/mol	McGowan Method
rinpol	3360.60		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U412610&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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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