(2E,10E)-11-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin

Inchi: InChI=1S/C23H31NO3/c25-23(24-16-10-7-11-17-24)13-9-6-4-2-1-3-5-8-12-20-14-15-21-
InchiKey: CHOLQJRIMZGPNC-QHKWOANTSA-N
Formula: C23H31NO3
SMILES: O=C(C=CCCCCCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 369.50
CAS: 807618-21-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.46		Crippen Method
logp	5.338		Crippen Method
mcvol	304.140	ml/mol	McGowan Method
rinpol	3427.20		NIST Webbook
rinpol	3427.20		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C807618219&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
rinpol: Non-polar retention indices