(E)-9-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)n

Inchi: InChI=1S/C21H29NO3/c23-21(22-14-8-5-9-15-22)11-7-4-2-1-3-6-10-18-12-13-19-20(16-
InchiKey: FAXXHNWVMKTOFF-UXBLZVDNSA-N
Formula: C21H29NO3
SMILES: O=C(CCCCCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 343.46
CAS: 30505-89-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.77		Crippen Method
logp	4.782		Crippen Method
mcvol	280.260	ml/mol	McGowan Method
rinpol	3159.00		NIST Webbook
rinpol	3159.00		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=C30505896&Units=SI

Legend

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