(2E,4E,6E)-7-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidi

Inchi: InChI=1S/C19H21NO3/c21-19(20-12-6-3-7-13-20)9-5-2-1-4-8-16-10-11-17-18(14-16)23-
InchiKey: DLKOUKNODPCIHZ-UMYWTXKFSA-N
Formula: C19H21NO3
SMILES: O=C(C=CC=CC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 311.37
CAS: 583-34-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.64		Crippen Method
logp	3.553		Crippen Method
mcvol	243.480	ml/mol	McGowan Method
rinpol	3209.00		NIST Webbook
rinpol	3272.90		NIST Webbook
rinpol	3209.00		NIST Webbook
rinpol	3272.90		NIST Webbook

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C583346&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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