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

Inchi: InChI=1S/C17H21NO3/c19-17(18-10-4-1-5-11-18)7-3-2-6-14-8-9-15-16(12-14)21-13-20-
InchiKey: MJBOPSKIWRUIBB-NSCUHMNNSA-N
Formula: C17H21NO3
SMILES: O=C(CC=CCc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 287.35
CAS: 23512-55-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.93		Crippen Method
logp	2.917		Crippen Method
mcvol	223.900	ml/mol	McGowan Method
rinpol	2601.80		NIST Webbook
rinpol	2601.80		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C23512552&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