

(Z)-5-(Benzo[d][1,3]dioxol-5-yl)-1-(piperidin-1-yl)po

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-IHWYPQMZSA-N
Formula: C17H21NO3
SMILES: O=C(CC=CCc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 287.35
CAS: 896710-01-3

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	2599.30		NIST Webbook
rinpol	2599.30		NIST Webbook

Sources

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=C896710013&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/118-431-2/Z-5-Benzo-d-1-3-dioxol-5-yl-1-piperidin-1-yl-pent-3-en-1-one.pdf>

Generated by Cheméo on 2024-04-23 19:25:31.044270155 +0000 UTC m=+16189579.964847467.
Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.