(E)-7-(Benzo[d][1,3]dioxol-5-yl)-1-(pyrrolidin-1-yl)h

Inchi: InChI=1S/C18H23NO3/c20-18(19-11-5-6-12-19)8-4-2-1-3-7-15-9-10-16-17(13-15)22-14-
InchiKey: UUHCCOYKUNWUQJ-XVNBXDOJSA-N
Formula: C18H23NO3
SMILES: O=C(CCCCC=Cc1ccc2c(c1)OCO2)N1CCCC1
Mol. weight [g/mol]: 301.38
CAS: 117137-66-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	3.611		Crippen Method
mcvol	237.990	ml/mol	McGowan Method

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=C117137663&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume