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

Inchi: InChI=1S/C20H27NO3/c22-20(21-13-7-8-14-21)10-6-4-2-1-3-5-9-17-11-12-18-19(15-17)
InchiKey: VBHDFZGBKBFFDM-WEVVVXLNSA-N
Formula: C20H27NO3
SMILES: O=C(CCCCCCC=Cc1ccc2c(c1)OCO2)N1CCCC1
Mol. weight [g/mol]: 329.43
CAS: 62510-52-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.35		Crippen Method
logp	4.392		Crippen Method
mcvol	266.170	ml/mol	McGowan Method
rinpol	3100.20		NIST Webbook
rinpol	3100.20		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C62510525&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