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

Inchi: InChI=1S/C19H25NO3/c21-19(20-12-6-3-7-13-20)9-5-2-1-4-8-16-10-11-17-18(14-16)23-
InchiKey: MIWPBXQTBYPJEF-XBXARRHUSA-N
Formula: C19H25NO3
SMILES: O=C(CCCCC=Cc1ccc2c(c1)OCO2)N1CCCCC1
Mol. weight [g/mol]: 315.41
CAS: 30505-92-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.93		Crippen Method
logp	4.001		Crippen Method
mcvol	252.080	ml/mol	McGowan Method
rinpol	2836.00		NIST Webbook
rinpol	2934.70		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C30505921&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