1,2-Propanediol, 3-(1-piperidinyl)-, bis(phenylcarbamate)

Other names: Diperodon
Inchi: InChI=1S/C22H27N3O4/c26-21(23-18-10-4-1-5-11-18)28-17-20(16-25-14-8-3-9-15-25)29
InchiKey: YUGZHQHSNYIFLG-UHFFFAOYSA-N
Formula: C22H27N3O4
SMILES: OC(=Nc1ccccc1)OCC(CN1CCCCC1)OC(O)=Nc1ccccc1
Mol. weight [g/mol]: 397.47
CAS: 101-08-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.15		Crippen Method
logp	4.366		Crippen Method
mcvol	307.280	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C101086&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