

1,2-Propanediol, 3-(1-piperidinyI)-, 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)2
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/ci9903071
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

Latest version available from:

<https://www.chemeo.com/cid/96-180-6/1-2-Propanediol-3-1-piperidinyI-bis-phenylcarbamate.pdf>

Generated by Cheméo on 2024-04-27 17:56:16.006135506 +0000 UTC m=+16529824.926712883.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.