(2-Hydroxy-3-phenyl-1,2-dihydroquinoxalin-1-yl)p

Inchi: InChI=1S/C42H34N4O/c47-42-39(32-21-9-3-10-22-32)44-35-26-14-16-28-37(35)46(42)4
InchiKey: SPVCYXNEMUPGJB-UHFFFAOYSA-N
Formula: C42H34N4O
SMILES: OC1C(c2ccccc2)=Nc2ccccc2N1C(c1ccccc1)C1C(c2ccccc2)=Nc2ccccc2N1Cc1ccccc1
Mol. weight [g/mol]: 610.75
CAS: 91757-02-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.62		Crippen Method
logp	8.897		Crippen Method
mcvol	475.550	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C91757027&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