2-(P-dodecylphenoxy) pyrazine

Inchi: InChI=1S/C22H32N2O/c1-2-3-4-5-6-7-8-9-10-11-12-20-13-15-21(16-14-20)25-22-19-23-
InchiKey: MLOJPIGVCAHKEM-UHFFFAOYSA-N
Formula: C22H32N2O
SMILES: CCCCCCCCCCCCc1ccc(Oc2cnccn2)cc1
Mol. weight [g/mol]: 340.50
CAS: 116660-31-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.63		Crippen Method
logp	6.732		Crippen Method
mcvol	299.150	ml/mol	McGowan Method

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660312&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume