2-(P-nonylphenoxy)-3-(p-phenoxybenzyl) pyrazine

Inchi: InChI=1S/C32H36N2O2/c1-2-3-4-5-6-7-9-12-26-15-19-30(20-16-26)36-32-31(33-23-24-3

InchiKey: QHGGSDYGTUIUPI-UHFFFAOYSA-N

Formula: C32H36N2O2

SMILES: CCCCCCCCCc1ccc(Oc2nccnc2Cc2ccc(Oc3ccccc3)cc2)cc1

Mol. weight [g/mol]: 480.64

CAS: 116402-78-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.11		Crippen Method
logp	8.945		Crippen Method
mcvol	398.400	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402789&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume