2-(P-nonylphenoxy)-3-(2-phenylethyl) pyrazine

Inchi: InChI=1S/C27H34N2O/c1-2-3-4-5-6-7-9-14-24-15-18-25(19-16-24)30-27-26(28-21-22-29
InchiKey: DPIKCIFLVRQVPG-UHFFFAOYSA-N
Formula: C27H34N2O
SMILES: CCCCCCCCCc1ccc(Oc2nccnc2CCc2ccccc2)cc1
Mol. weight [g/mol]: 402.57
CAS: 116402-94-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.79		Crippen Method
logp	7.347		Crippen Method
mcvol	345.840	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=C116402949&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