2-(P-nonylphenoxy)-6-(2-phenylethyl) pyrazine

Inchi: InChI=1S/C27H34N2O/c1-2-3-4-5-6-7-9-14-24-16-19-26(20-17-24)30-27-22-28-21-25(29
InchiKey: OCHCRLPYOHUGNA-UHFFFAOYSA-N
Formula: C27H34N2O
SMILES: CCCCCCCCCc1ccc(Oc2cncc(CCc3ccccc3)n2)cc1
Mol. weight [g/mol]: 402.57
CAS: 116402-77-8

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: 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=C116402778&Units=SI

Legend

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