2-(P-nonylphenoxy)-3-methyl-6-(2-phenylethyl) pyrazine

Inchi: InChI=1S/C28H36N2O/c1-3-4-5-6-7-8-10-15-25-17-20-27(21-18-25)31-28-23(2)29-22-26

InchiKey: HIENIMGBZJFVKK-UHFFFAOYSA-N

Formula: C28H36N2O

SMILES: CCCCCCCCCc1ccc(Oc2nc(CCc3ccccc3)cnc2C)cc1

Mol. weight [g/mol]: 416.60

Physical Properties

Property code	Value	Unit	Source
log10ws	-9.26		Crippen Method
logp	7.656		Crippen Method
mcvol	359.930	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003115&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