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

Inchi: InChI=1S/C27H34N2O/c1-3-4-5-6-7-8-10-13-23-16-18-26(19-17-23)30-27-22(2)28-21-25

InchiKey: BERFGWOXHRCHLZ-UHFFFAOYSA-N

Formula: C27H34N2O

SMILES: CCCCCCCCCc1ccc(Oc2nc(Cc3ccccc3)cnc2C)cc1

Mol. weight [g/mol]: 402.57

CAS: 116402-76-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.95		Crippen Method
logp	7.461		Crippen Method
mcvol	345.840	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402767&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