

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

McGowan Method: <http://link.springer.com/article/10.1007/BF02311772>
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

Legend

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

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