2-(P-nonylphenoxy)-3-methyl-6-(5-nonyl) pyrazine

Inchi: InChI=1S/C29H46N2O/c1-5-8-11-12-13-14-15-16-25-19-21-27(22-20-25)32-29-24(4)30-2

InchiKey: ZNUOKLVLLDFYRI-UHFFFAOYSA-N

Formula: C29H46N2O

SMILES: CCCCCCCCCc1ccc(Oc2nc(C(CCCC)CCCC)cnc2C)cc1

Mol. weight [g/mol]: 438.69

CAS: 116402-96-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.54		Crippen Method
logp	9.334		Crippen Method
mcvol	397.780	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402961&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