

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

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