2-(P-nonylphenoxy)-3-(n-pentyl)-6-(5-nonyl) pyrazine

Inchi: InChI=1S/C33H54N2O/c1-5-9-13-14-15-16-18-19-28-23-25-30(26-24-28)36-33-31(22-17

InchiKey: VPKTYKKCTNBEGU-UHFFFAOYSA-N

Formula: C33H54N2O

SMILES: CCCCCCCCCc1ccc(Oc2nc(C(CCCC)CCCC)cnc2CCCCC)cc1

Mol. weight [g/mol]: 494.79

CAS: 116402-98-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.13		Crippen Method
logp	10.759		Crippen Method
mcvol	454.140	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=C116402983&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