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

Inchi: InChI=1S/C33H54N2O/c1-4-6-8-10-12-13-14-15-17-19-21-23-31-28-34-29(3)33(35-31)36

InchiKey: QDOASHAXZZEMKB-UHFFFAOYSA-N

Formula: C33H54N2O

SMILES: CCCCCCCCCCCCCc1cnc(C)c(Oc2ccc(CCCCCCCCC)cc2)n1

Mol. weight [g/mol]: 494.79

Physical Properties

Property code	Value	Unit	Source
log10ws	-12.25		Crippen Method
logp	10.724		Crippen Method
mcvol	454.140	ml/mol	McGowan Method

Sources

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=B6003123&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume