

2-(P-nonylphenoxy)-3-methyl-6-tridecylpyrazine

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)3
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

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