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

Inchi: InChI=1S/C32H52N2O/c1-3-5-7-9-11-12-13-14-16-18-20-22-30-27-33-28-32(34-30)35-31
InchiKey: YPHJBHBGEWQPLA-UHFFFAOYSA-N
Formula: C32H52N2O
SMILES: CCCCCCCCCCCCCc1cncc(Oc2ccc(CCCCCCCCC)cc2)n1
Mol. weight [g/mol]: 480.77
CAS: 116403-08-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-11.78		Crippen Method
logp	10.415		Crippen Method
mcvol	440.050	ml/mol	McGowan Method

Sources

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=C116403088&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume