2-(P-nonylphenoxy)-3-methyl-6-(p-phenoxybenzyl

Inchi: InChI=1S/C33H38N2O2/c1-3-4-5-6-7-8-10-13-27-16-20-32(21-17-27)37-33-26(2)34-25-2
InchiKey: BRLUUQMJOONIHY-UHFFFAOYSA-N
Formula: C33H38N2O2
SMILES: CCCCCCCCCc1ccc(Oc2nc(Cc3ccc(Oc4ccccc4)cc3)cnc2C)cc1
Mol. weight [g/mol]: 494.67
CAS: 116402-89-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.58		Crippen Method
logp	9.254		Crippen Method
mcvol	412.490	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=C116402892&Units=SI

Legend

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