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:	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
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

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