

2-(P-nonylphenoxy)-6-(p-phenoxybenzyl)pyrazine

Inchi:	InChI=1S/C32H36N2O2/c1-2-3-4-5-6-7-9-13-26-18-20-30(21-19-26)36-32-25-33-24-28(3
InchiKey:	BPQRUMNLTOSWOV-UHFFFAOYSA-N
Formula:	C32H36N2O2
SMILES:	CCCCCCCCc1ccc(Oc2cncc(Cc3cccc(Oc4cccc4)c3)n2)cc1
Mol. weight [g/mol]:	480.64

Physical Properties

Property code	Value	Unit	Source
log10ws	-10.11		Crippen Method
logp	8.945		Crippen Method
mcvol	398.400	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=B6003139&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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