

2-(P-phenylphenoxy)-3-(5-nonyl) pyrazine

Inchi:	InChI=1S/C25H30N2O/c1-3-5-10-22(11-6-4-2)24-25(27-19-18-26-24)28-23-16-14-21(15-
InchiKey:	NYLWFRPEGAQURW-UHFFFAOYSA-N
Formula:	C25H30N2O
SMILES:	CCCCC(CCCC)c1nccnc1Oc1ccc(-c2ccccc2)cc1
Mol. weight [g/mol]:	374.52
CAS:	116660-12-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.94		Crippen Method
logp	7.400		Crippen Method
mcvol	317.660	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=C116660129&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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