

2-(M-phenoxyphenoxy)-3-(5-nonyl) pyrazine

Inchi:	InChI=1S/C25H30N2O2/c1-3-5-11-20(12-6-4-2)24-25(27-18-17-26-24)29-23-16-10-15-22
InchiKey:	KSKHJBNVZKHJIG-UHFFFAOYSA-N
Formula:	C25H30N2O2
SMILES:	CCCCC(CCCC)c1nccnc1Oc1cccc(Oc2ccccc2)c1
Mol. weight [g/mol]:	390.52
CAS:	5008-88-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.97		Crippen Method
logp	7.525		Crippen Method
mcvol	323.530	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C5008888&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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