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