2-(2-Methyl-6-ethylphenoxy)-3-(5-nonyl) pyrazine

Inchi: InChI=1S/C22H32N2O/c1-5-8-12-19(13-9-6-2)20-22(24-16-15-23-20)25-21-17(4)11-10-1

InchiKey: CROZTSWLMFSIDN-UHFFFAOYSA-N

Formula: C22H32N2O

SMILES: CCCCC(CCCC)c1nccnc1Oc1c(C)cccc1CC

Mol. weight [g/mol]: 340.50

CAS: 116668-93-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.61		Crippen Method
logp	6.604		Crippen Method
mcvol	299.150	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=C116668930&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