

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: CROZTSWLMFSDN-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/ci9903071>

Legend

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

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