2-(P-nonylphenoxy)-3,6-dimethyl pyrazine

Inchi: InChI=1S/C21H30N2O/c1-4-5-6-7-8-9-10-11-19-12-14-20(15-13-19)24-21-18(3)22-16-17
InchiKey: VGRZBOZMQBSNEV-UHFFFAOYSA-N
Formula: C21H30N2O
SMILES: CCCCCCCCCc1ccc(Oc2nc(C)cnc2C)cc1
Mol. weight [g/mol]: 326.48
CAS: 116660-22-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.32		Crippen Method
logp	6.179		Crippen Method
mcvol	285.060	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=C116660221&Units=SI

Legend

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