

2-(P-nonylphenoxy)-3-methyl pyrazine

InChI: InChI=1S/C20H28N2O/c1-3-4-5-6-7-8-9-10-18-11-13-19(14-12-18)
23-20-17(2)21-15-16-22-20/h11-16H,3-10H2,1-2H3

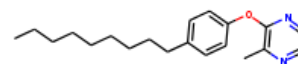
InChI Key: MIFCXYCKDIHAKQ-UHFFFAOYSA-N

Formula: C20H28N2O

SMILES: CCCCCCCCc1ccc(Oc2nccnc2C)cc1

Molecular Weight: 312.45

CAS: 116660-49-2



Physical Properties

Property	Value	Unit	Source
$\log P_{\text{oct/wat}}$	5.87		Crippen Method

Sources

NIST Webbook: [http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28N2O/c1-3-4-5-6-7-8-9-10-18-11-13-19\(14-12-18\)23-20-17\(2\)21-15-16-22-20/h11-16H,3-10H2,1-2H3](http://webbook.nist.gov/cgi/inchi/InChI=1S/C20H28N2O/c1-3-4-5-6-7-8-9-10-18-11-13-19(14-12-18)23-20-17(2)21-15-16-22-20/h11-16H,3-10H2,1-2H3)

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

$\log P_{\text{oct/wat}}$: Octanol/Water partition coefficient .

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