2-(P-nonylphenoxy) pyrazine

Inchi:	InChI=1S/C19H26N2O/c1-2-3-4-5-6-7-8-9-17-10-12-18(13-11-17)22-19-16-20-14-15-21-
InchiKey:	PGRRFTMMIQTILZ-UHFFFAOYSA-N
Formula:	C19H26N2O
SMILES:	CCCCCCCCCc1ccc(Oc2cnccn2)cc1
Mol. weight [g/mol]:	298.42
CAS:	116659-78-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	5.562		Crippen Method
mcvol	256.880	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=C116659780&Units=SI

Legend

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

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