2-Phenoxy-3-(5-nonyl) pyrazine

Inchi:	InChI=1S/C19H26N2O/c1-3-5-10-16(11-6-4-2)18-19(21-15-14-20-18)22-17-12-8-7-9-13-
InchiKey:	REXJSXHTXGTZTJ-UHFFFAOYSA-N
Formula:	C19H26N2O
SMILES:	CCCCC(CCCC)c1nccnc1Oc1ccccc1
Mol. weight [g/mol]:	298.42
CAS:	5008-87-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.33		Crippen Method
logp	5.733		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=C5008877&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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