

2-(O-phenylphenoxy) pyrazine

Inchi:	InChI=1S/C16H12N2O/c1-2-6-13(7-3-1)14-8-4-5-9-15(14)19-16-12-17-10-11-18-16/h1-1
InchiKey:	CHFDNBAZVGQWTL-UHFFFAOYSA-N
Formula:	C16H12N2O
SMILES:	c1ccc(-c2ccccc2Oc2cnccn2)cc1
Mol. weight [g/mol]:	248.28
CAS:	116435-19-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.24		Crippen Method
logp	3.936		Crippen Method
mcvol	190.850	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435199&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/29-416-8/2-O-phenylphenoxy-pyrazine.pdf>

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