

2-Phenoxy-3-(p-phenoxy benzyl) pyrazine

Inchi:	InChI=1S/C23H18N2O2/c1-3-7-19(8-4-1)26-21-13-11-18(12-14-21)17-22-23(25-16-15-24)
InchiKey:	DLXATDXPFDTLJF-UHFFFAOYSA-N
Formula:	C23H18N2O2
SMILES:	c1ccc(Oc2ccc(Cc3nccnc3Oc3ccccc3)cc2)cc1
Mol. weight [g/mol]:	354.40
CAS:	116659-45-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	5.652		Crippen Method
mcvol	271.590	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=C116659451&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

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<https://www.chemeo.com/cid/97-318-2/2-Phenoxy-3-p-phenoxy-benzyl-pyrazine.pdf>

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