2-Phenoxy-3-methyl-6-benzyl pyrazine

Inchi:	InChI=1S/C18H16N2O/c1-14-18(21-17-10-6-3-7-11-17)20-16(13-19-14)12-15-8-4-2-5-9-
InchiKey:	JFGMPTAICVEAKY-UHFFFAOYSA-N
Formula:	C18H16N2O
SMILES:	Cc1ncc(Cc2ccccc2)nc1Oc1ccccc1
Mol. weight [g/mol]:	276.33
CAS:	116435-99-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.168		Crippen Method
mcvol	219.030	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116435995&Units=SI
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

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/99-281-1/2-Phenoxy-3-methyl-6-benzyl-pyrazine.pdf

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