

2-Phenoxy-3-benzyl pyrazine

Inchi:	InChI=1S/C17H14N2O/c1-3-7-14(8-4-1)13-16-17(19-12-11-18-16)20-15-9-5-2-6-10-15/h
InchiKey:	CGIDEQICOWXIDQ-UHFFFAOYSA-N
Formula:	C17H14N2O
SMILES:	c1ccc(Cc2nccnc2Oc2ccccc2)cc1
Mol. weight [g/mol]:	262.31
CAS:	116435-98-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.860		Crippen Method
mcvol	204.940	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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=C116435984&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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<https://www.chemeo.com/cid/44-054-3/2-Phenoxy-3-benzyl-pyrazine.pdf>

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