

2-Phenoxy-6-benzyl pyrazine

Inchi:	InChI=1S/C17H14N2O/c1-3-7-14(8-4-1)11-15-12-18-13-17(19-15)20-16-9-5-2-6-10-16/h
InchiKey:	PXJUHRHBCOXEHN-UHFFFAOYSA-N
Formula:	C17H14N2O
SMILES:	c1ccc(Cc2cncc(Oc3ccccc3)n2)cc1
Mol. weight [g/mol]:	262.31
CAS:	116660-05-0

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:	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=C116660050&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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