

2-Phenoxy-6-benzoyl pyrazine

Inchi:	InChI=1S/C17H12N2O2/c20-17(13-7-3-1-4-8-13)15-11-18-12-16(19-15)21-14-9-5-2-6-10
InchiKey:	KIZJWFCCYFLLIR-UHFFFAOYSA-N
Formula:	C17H12N2O2
SMILES:	O=C(c1ccccc1)c1cncc(Oc2ccccc2)n1
Mol. weight [g/mol]:	276.29
CAS:	116659-99-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.60		Crippen Method
logp	3.500		Crippen Method
mcvol	206.510	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=C116659995&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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/23-766-6/2-Phenoxy-6-benzoyl-pyrazine.pdf>

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