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/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