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/h1
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/ci990307l
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