2-Phenoxy-3-(2-phenyl ethyl) pyrazine

Inchi: InChI=1S/C18H16N2O/c1-3-7-15(8-4-1)11-12-17-18(20-14-13-19-17)21-16-9-5-2-6-10-1
InchiKey: DFYRUZZLUBPDNB-UHFFFAOYSA-N
Formula: C18H16N2O
SMILES: c1ccc(CCc2nccnc2Oc2ccccc2)cc1
Mol. weight [g/mol]: 276.33
CAS: 116659-83-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.06		Crippen Method
logp	4.054		Crippen Method
mcvol	219.030	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=C116659837&Units=SI

Legend

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