2-Phenoxy-3-(p-phenoxy benzyl) pyrazine

Inchi: InChI=1S/C23H18N2O2/c1-3-7-19(8-4-1)26-21-13-11-18(12-14-21)17-22-23(25-16-15-24
InchiKey: DLXATDXPFDTLJF-UHFFFAOYSA-N
Formula: C23H18N2O2
SMILES: c1ccc(Oc2ccc(Cc3nccnc3Oc3ccccc3)cc2)cc1
Mol. weight [g/mol]: 354.40
CAS: 116659-45-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.37		Crippen Method
logp	5.652		Crippen Method
mcvol	271.590	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=C116659451&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