2-Phenoxy-3-benzhydryl pyrazine

Inchi: InChI=1S/C23H18N2O/c1-4-10-18(11-5-1)21(19-12-6-2-7-13-19)22-23(25-17-16-24-22)2
InchiKey: XLFMCYIPOLJGFG-UHFFFAOYSA-N
Formula: C23H18N2O
SMILES: c1ccc(Oc2nccnc2C(c2ccccc2)c2ccccc2)cc1
Mol. weight [g/mol]: 338.40
CAS: 116660-30-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.42		Crippen Method
logp	5.449		Crippen Method
mcvol	265.720	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660301&Units=SI
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

Legend

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