2-Phenoxy-3-tridecyl pyrazine

Inchi: InChI=1S/C23H34N2O/c1-2-3-4-5-6-7-8-9-10-11-15-18-22-23(25-20-19-24-22)26-21-16-
InchiKey: DDJCJUNERJIMJL-UHFFFAOYSA-N
Formula: C23H34N2O
SMILES: CCCCCCCCCCCCCc1nccnc1Oc1ccccc1
Mol. weight [g/mol]: 354.53
CAS: 116659-46-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.05		Crippen Method
logp	7.122		Crippen Method
mcvol	313.240	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116659462&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