2-Phenoxy-3,6-dimethyl pyrazine

Inchi: InChI=1S/C12H12N2O/c1-9-8-13-10(2)12(14-9)15-11-6-4-3-5-7-11/h3-8H,1-2H3
InchiKey: XHMYGFGJEPCOIE-UHFFFAOYSA-N
Formula: C12H12N2O
SMILES: Cc1cnc(C)c(Oc2ccccc2)n1
Mol. weight [g/mol]: 200.24
CAS: 116660-24-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.59		Crippen Method
logp	2.886		Crippen Method
mcvol	158.250	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=C116660243&Units=SI

Legend

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