

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:	XHMYGFGJEP COIE-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/ci9903071
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

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<https://www.chemeo.com/cid/25-315-4/2-Phenoxy-3-6-dimethyl-pyrazine.pdf>

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