

2-(2,2-Dimethylpentoxy)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C13H22N2O/c1-6-7-13(4,5)9-16-12-11(3)14-8-10(2)15-12/h8H,6-7,9H2,1-5H3
InchiKey:	DSEGKKGZERLGYFB-UHFFFAOYSA-N
Formula:	C13H22N2O
SMILES:	CCCC(C)(C)COc1nc(C)cnc1C
Mol. weight [g/mol]:	222.33
CAS:	116660-21-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.34		Crippen Method
logp	3.299		Crippen Method
mcvol	196.100	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=C116660210&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
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

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<https://www.chemeo.com/cid/13-142-9/2-2-2-Dimethylpentoxy-3-6-dimethyl-pyrazine.pdf>

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