

# 2-(2,2,4-Trimethylpentoxy)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C14H24N2O/c1-10(2)7-14(5,6)9-17-13-12(4)15-8-11(3)16-13/h8,10H,7,9H2,1-
InchiKey:	HWVHYMQSPCNBIT-UHFFFAOYSA-N
Formula:	C14H24N2O
SMILES:	Cc1cnc(C)c(OCC(C)(C)CC(C)C)n1
Mol. weight [g/mol]:	236.35
CAS:	116660-26-5

## Physical Properties

Property code	Value	Unit	Source
log10ws	-4.52		Crippen Method
logp	3.545		Crippen Method
mcvol	210.190	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660265&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116660265&amp;Units=SI</a>
Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>

## Legend

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

Latest version available from:

<https://www.chemeo.com/cid/121-037-6/2-2-2-4-Trimethylpentoxy-3-6-dimethyl-pyrazine.pdf>

Generated by Cheméo on 2024-05-02 00:44:23.168406981 +0000 UTC m=+16899912.088984292.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.