

2-(2,2-Dimethylpentoxy)-3-methyl-6-(n-pentyl)pyrazine

Inchi:	InChI=1S/C17H30N2O/c1-6-8-9-10-15-12-18-14(3)16(19-15)20-13-17(4,5)11-7-2/h12H,6
InchiKey:	RQHMRSCRXRPLH-UHFFFAOYSA-N
Formula:	C17H30N2O
SMILES:	CCCCC1cnc(C)c(OCC(C)(C)CCC)n1
Mol. weight [g/mol]:	278.43
CAS:	116668-94-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.93		Crippen Method
logp	4.723		Crippen Method
mcvol	252.460	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C116668941&Units=SI
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

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/13-345-4/2-2-2-Dimethylpentoxy-3-methyl-6-n-pentyl-pyrazine.pdf>

Generated by Cheméo on 2024-04-23 13:05:18.72141668 +0000 UTC m=+16166767.641993992.

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