

2-(2,2,4-Trimethylpentoxy)-3-(n-pentyl)pyrazine

Inchi:	InChI=1S/C17H30N2O/c1-6-7-8-9-15-16(19-11-10-18-15)20-13-17(4,5)12-14(2)3/h10-11
InchiKey:	WBRJSGNTCBKXBR-UHFFFAOYSA-N
Formula:	C17H30N2O
SMILES:	CCCCC1nccnc1OCC(C)(C)CC(C)C
Mol. weight [g/mol]:	278.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.63		Crippen Method
logp	4.660		Crippen Method
mcvol	252.460	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=B6003302&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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