2-(2,2,4-Trimethylpentoxy)-3-(5-nonyl) pyrazine

Inchi:	InChI=1S/C21H38N2O/c1-7-9-11-18(12-10-8-2)19-20(23-14-13-22-19)24-16-21(5,6)15-1
InchiKey:	KIQIDZVMOAZCAG-UHFFFAOYSA-N
Formula:	C21H38N2O
SMILES:	CCCCC(CCCC)c1nccnc1OCC(C)(C)CC(C)C
Mol. weight [g/mol]:	334.54
CAS:	5008-90-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.27		Crippen Method
logp	6.392		Crippen Method
mcvol	308.820	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C5008902&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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