

2-(2,2,4-Trimethylpentoxy)-3-methyl pyrazine

Inchi:	InChI=1S/C13H22N2O/c1-10(2)8-13(4,5)9-16-12-11(3)14-6-7-15-12/h6-7,10H,8-9H2,1-5
InchiKey:	MABUKNLWUYRSSQ-UHFFFAOYSA-N
Formula:	C13H22N2O
SMILES:	Cc1nccnc1OCC(C)(C)CC(C)C
Mol. weight [g/mol]:	222.33
CAS:	116659-77-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.05		Crippen Method
logp	3.236		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=C116659779&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/122-222-9/2-2-2-4-Trimethylpentoxy-3-methyl-pyrazine.pdf>

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