

2-(2,2-Dimethylpentoxy)-3-(5-nonyl) pyrazine

Inchi:	InChI=1S/C20H36N2O/c1-6-9-11-17(12-10-7-2)18-19(22-15-14-21-18)23-16-20(4,5)13-8
InchiKey:	XTIHPGCNUNGKGZ-UHFFFAOYSA-N
Formula:	C20H36N2O
SMILES:	CCCCC(CCCC)c1nccnc1OCC(C)(C)CCC
Mol. weight [g/mol]:	320.51
CAS:	2850-79-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.09		Crippen Method
logp	6.146		Crippen Method
mcvol	294.730	ml/mol	McGowan Method

Sources

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=C2850795&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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