

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

InChI:	InChI=1S/C23H42N2O/c1-6-9-11-12-14-15-20-18-24-21(16-13-10-7-2)22(25-20)26-19-23
InChIKey:	WJWWWDDDILISTJ-UHFFFAOYSA-N
Formula:	C23H42N2O
SMILES:	CCCCCCCc1cnc(CCCCC)c(OCC(C)(C)CCC)n1
Mol. weight [g/mol]:	362.59
CAS:	3049-56-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.35		Crippen Method
logp	6.927		Crippen Method
mcvol	337.000	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C3049567&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

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