

# 2-(N,n-di-n-butyl amino)-3-(5-nonyl) pyrazine

<b>Inchi:</b>	InChI=1S/C21H39N3/c1-5-9-13-19(14-10-6-2)20-21(23-16-15-22-20)24(17-11-7-3)18-12
<b>InchiKey:</b>	SKKMXBNBGMROJE-UHFFFAOYSA-N
<b>Formula:</b>	C21H39N3
<b>SMILES:</b>	CCCC(CCCC)c1nccnc1N(CCCC)CCCC
<b>Mol. weight [g/mol]:</b>	333.55
<b>CAS:</b>	116402-95-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-7.12		Crippen Method
logp	6.347		Crippen Method
mcvol	312.930	ml/mol	McGowan Method

## Sources

<b>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402950&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402950&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>

## Legend

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

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