

# 2-(N-n-hexyl-n-n-octylamino)-3-(n-nonyl)pyrazine

Inchi:	InChI=1S/C27H51N3/c1-4-7-10-13-15-16-18-21-26-27(29-23-22-28-26)30(24-19-12-9-6-
InchiKey:	XVIMFVWRVKCNMT-UHFFFAOYSA-N
Formula:	C27H51N3
SMILES:	CCCCCCCCc1nccnc1N(CCCCC)CCCCCCC
Mol. weight [g/mol]:	417.71
CAS:	116402-86-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-9.67		Crippen Method
logp	8.517		Crippen Method
mcvol	397.470	ml/mol	McGowan Method

## Sources

Crippen Method:	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
Crippen Method:	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>
McGowan Method:	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
NIST Webbook:	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402869&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402869&amp;Units=SI</a>

## Legend

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

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