

2-(N-pentyl)-6-(5-nonyl) pyrazine

Inchi:	InChI=1S/C18H32N2/c1-4-7-10-13-17-14-19-15-18(20-17)16(11-8-5-2)12-9-6-3/h14-16H
InchiKey:	CTELUPPQUSAMGW-UHFFFAOYSA-N
Formula:	C18H32N2
SMILES:	CCCCC1CNCC(C(CCCC)CCCC)n1
Mol. weight [g/mol]:	276.46
CAS:	131346-15-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.76		Crippen Method
logp	5.673		Crippen Method
mcvol	260.680	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=C131346151&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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