2-(N,n-di-n-pentylamino)-3-methyl pyrazine

Inchi:	InChI=1S/C15H27N3/c1-4-6-8-12-18(13-9-7-5-2)15-14(3)16-10-11-17-15/h10-11H,4-9,12
InchiKey:	HZSMNLROZUIKRE-UHFFFAOYSA-N
Formula:	C15H27N3
SMILES:	CCCCCN(CCCCC)c1nccnc1C
Mol. weight [g/mol]:	249.40
CAS:	116660-29-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.74		Crippen Method
logp	3.972		Crippen Method
mcvol	228.390	ml/mol	McGowan Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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=C116660298&Units=SI

Legend

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

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