

3-(N,n-di-n-pentylamino)-2,5-dimethyl pyrazine

Inchi:	InChI=1S/C16H29N3/c1-5-7-9-11-19(12-10-8-6-2)16-15(4)17-13-14(3)18-16/h13H,5-12H
InchiKey:	XQRCSOJPRNXZTG-UHFFFAOYSA-N
Formula:	C16H29N3
SMILES:	CCCCCN(CCCCC)c1nc(C)cnc1C
Mol. weight [g/mol]:	263.42
CAS:	116402-81-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.280		Crippen Method
mcvol	242.480	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=C116402814&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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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