

2-(N,n-di-n-butylamino)-3-(n-pentyl)pyrazine

Inchi:	InChI=1S/C17H31N3/c1-4-7-10-11-16-17(19-13-12-18-16)20(14-8-5-2)15-9-6-3/h12-13H
InchiKey:	XKSHZBQNXPLKOP-UHFFFAOYSA-N
Formula:	C17H31N3
SMILES:	CCCCC1nccnc1N(CCCC)CCCC
Mol. weight [g/mol]:	277.45
CAS:	116403-00-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.48		Crippen Method
logp	4.616		Crippen Method
mcvol	256.570	ml/mol	McGowan Method

Sources

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=C116403000&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

Legend

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

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