

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

Inchi:	InChI=1S/C13H23N3/c1-4-6-10-16(11-7-5-2)13-12(3)14-8-9-15-13/h8-9H,4-7,10-11H2,1-
InchiKey:	ZTGXZXCXJPOQAI-UHFFFAOYSA-N
Formula:	C13H23N3
SMILES:	CCCCN(CCCC)c1nccnc1C
Mol. weight [g/mol]:	221.34
CAS:	116660-17-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.90		Crippen Method
logp	3.192		Crippen Method
mcvol	200.210	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=C116660174&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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

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