2-(N,n-diisobutylamino)-3,6-dimethyl pyrazine

Inchi:	InChI=1S/C14H25N3/c1-10(2)8-17(9-11(3)4)14-13(6)15-7-12(5)16-14/h7,10-11H,8-9H2,1
InchiKey:	CVOLUGBDLARELO-UHFFFAOYSA-N
Formula:	C14H25N3
SMILES:	Cc1cnc(C)c(N(CC(C)C)CC(C)C)n1
Mol. weight [g/mol]:	235.37
CAS:	116660-19-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.89		Crippen Method
logp	3.212		Crippen Method
mcvol	214.300	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=C116660196&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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