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

Inchi: InChI=1S/C14H25N3/c1-5-7-9-17(10-8-6-2)14-13(4)15-11-12(3)16-14/h11H,5-10H2,1-4H
InchiKey: HFNGWNNJLWDPHQ-UHFFFAOYSA-N
Formula: C14H25N3
SMILES: CCCCN(CCCC)c1nc(C)cnc1C
Mol. weight [g/mol]: 235.37
CAS: 116660-16-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.37		Crippen Method
logp	3.500		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=C116660163&Units=SI

Legend

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