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