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

Inchi: InChI=1S/C17H31N3/c1-4-6-8-10-14-20(15-11-9-7-5-2)17-16(3)18-12-13-19-17/h12-13H
InchiKey: QJVHHAJJGUJWBI-UHFFFAOYSA-N
Formula: C17H31N3
SMILES: CCCCCCN(CCCCCC)c1nccnc1C
Mol. weight [g/mol]: 277.45
CAS: 116403-07-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.57		Crippen Method
logp	4.752		Crippen Method
mcvol	256.570	ml/mol	McGowan Method

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116403077&Units=SI
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

Legend

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