2-(N,n-di-n-pentyl amino)-3-(n-pentyl)pyrazine

Inchi: InChI=1S/C19H35N3/c1-4-7-10-13-18-19(21-15-14-20-18)22(16-11-8-5-2)17-12-9-6-3/h1
InchiKey: BNPQMZINFOJQHU-UHFFFAOYSA-N
Formula: C19H35N3
SMILES: CCCCCc1nccnc1N(CCCCC)CCCCC
Mol. weight [g/mol]: 305.50
CAS: 116402-84-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.32		Crippen Method
logp	5.396		Crippen Method
mcvol	284.750	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=C116402847&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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