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

Inchi: InChI=1S/C16H29N3/c1-5-7-9-11-19(12-10-8-6-2)16-15(4)17-13-14(3)18-16/h13H,5-12H
InchiKey: XQRCSOJPRNXZTG-UHFFFAOYSA-N
Formula: C16H29N3
SMILES: CCCCCN(CCCCC)c1nc(C)cnc1C
Mol. weight [g/mol]: 263.42
CAS: 116402-81-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.21		Crippen Method
logp	4.280		Crippen Method
mcvol	242.480	ml/mol	McGowan Method

Sources

McGowan Method: http://link.springer.com/article/10.1007/BF02311772
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402814&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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