2-(N-butyl-p-pentylanilino)-3-(n-pentyl) pyrazine

Inchi: InChI=1S/C24H37N3/c1-4-7-10-12-21-14-16-22(17-15-21)27(20-9-6-3)24-23(13-11-8-5-2
InchiKey: JKWMDVXPTOMPDN-UHFFFAOYSA-N
Formula: C24H37N3
SMILES: CCCCCc1ccc(N(CCCC)c2nccnc2CCCCC)cc1
Mol. weight [g/mol]: 367.57
CAS: 116403-09-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-8.08		Crippen Method
logp	6.880		Crippen Method
mcvol	331.440	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=C116403099&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

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