

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

Inchi: InChI=1S/C23H43N3/c1-4-7-10-13-14-17-22-23(25-19-18-24-22)26(20-15-11-8-5-2)21-1
InchiKey: PGXRBWGUGURHGK-UHFFFAOYSA-N
Formula: C23H43N3
SMILES: CCCCCCc1nccnc1N(CCCCCC)CCCCC
Mol. weight [g/mol]: 361.61
CAS: 116403-05-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.99		Crippen Method
logp	6.957		Crippen Method
mcvol	341.110	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C116403055&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

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