

2-(N-n-hexylanilino)-3-(n-heptyl) pyrazine

Inchi: InChI=1S/C23H35N3/c1-3-5-7-9-13-17-22-23(25-19-18-24-22)26(20-14-8-6-4-2)21-15-11
InchiKey: NTXXVHJIQAYFFQ-UHFFFAOYSA-N
Formula: C23H35N3
SMILES: CCCCCCc1nccnc1N(CCCCCC)c1cccc1
Mol. weight [g/mol]: 353.54
CAS: 131346-16-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.70		Crippen Method
logp	6.708		Crippen Method
mcvol	317.350	ml/mol	McGowan Method

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C131346162&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

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