

# 3-(N-methylanilino)-2-(n-pentyl)-5-(n-heptyl)pyrazine

|                      |                                                                                   |
|----------------------|-----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C23H35N3/c1-4-6-8-9-12-15-20-19-24-22(18-11-7-5-2)23(25-20)26(3)21-16-13 |
| InchiKey:            | QFNYGBRCCGYZQK-UHFFFAOYSA-N                                                       |
| Formula:             | C23H35N3                                                                          |
| SMILES:              | CCCCCCCCc1cnc(CCCCC)c(N(C)c2cccc2)n1                                              |
| Mol. weight [g/mol]: | 353.54                                                                            |
| CAS:                 | 116402-85-8                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -7.66   |        | Crippen Method |
| logp          | 6.490   |        | Crippen Method |
| mcvol         | 317.350 | ml/mol | McGowan Method |

## Sources

|                 |                                                                                                                                                 |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                               |
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                           |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402858&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402858&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                       |

## Legend

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

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