

2-(N-n-di-n-hexylamino)-3-(n-pentyl)-6-(n-heptyl)pyrazine

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|----------------------|--|
| InChI: | InChI=1S/C28H53N3/c1-5-9-13-16-18-21-26-25-29-27(22-17-12-8-4)28(30-26)31(23-19- |
| InChIKey: | IZPGULQMHORVJY-UHFFFAOYSA-N |
| Formula: | C28H53N3 |
| SMILES: | CCCCCCCc1cnc(CCCCC)c(N(CCCCC)CCCCC)n1 |
| Mol. weight [g/mol]: | 431.74 |
| CAS: | 116402-80-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| log10ws | -10.05 | | Crippen Method |
| logp | 8.689 | | Crippen Method |
| mcvol | 411.560 | ml/mol | McGowan Method |

Sources

| | |
|-----------------|---|
| 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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C116402803&Units=SI |

Legend

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

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