

# Acetanilide, N-(1-phenethyl-4-piperidyl)-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Acetamide, N-phenyl-N-[1-(2-phenylethyl)-4-piperidiny]-<br>Fentanyl acetyl analog<br>Acetyl fentanyl |
| <b>Inchi:</b>               | InChI=1S/C21H26N2O/c1-18(24)23(20-10-6-3-7-11-20)21-13-16-22(17-14-21)15-12-19-8                     |
| <b>InchiKey:</b>            | FYIUUQUPOKIKNI-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C21H26N2O  |
| <b>SMILES:</b>              | CC(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1  |
| <b>Mol. weight [g/mol]:</b> | 322.44   |
| <b>CAS:</b>                 | 3258-84-2  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -4.28   |        | Crippen Method |
| logp          | 3.747   |        | Crippen Method |
| mcvol         | 269.900 | ml/mol | McGowan Method |
| rinpol        | 2765.00 |        | NIST Webbook   |
| rinpol        | 2765.00 |        | NIST Webbook   |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3258842&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3258842&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                       |

## Legend

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>rinpol:</b>  | Non-polar retention indices         |

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