

# Methyl-3-fentanyl

|                      |                                                                                 |
|----------------------|---------------------------------------------------------------------------------|
| Other names:         | Butanoyl fentanyl                                                               |
| Inchi:               | InChI=1S/C23H30N2O/c1-2-9-23(26)25(21-12-7-4-8-13-21)22-15-18-24(19-16-22)17-14 |
| InchiKey:            | QQOMYEQLWQJRKK-UHFFFAOYSA-N                                                     |
| Formula:             | C23H30N2O                                                                       |
| SMILES:              | CCCC(=O)N(c1ccccc1)C1CCN(CCc2ccccc2)CC1                                         |
| Mol. weight [g/mol]: | 350.50                                                                          |
| CAS:                 | 1169-70-6                                                                       |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.11   |        | Crippen Method |
| logp          | 4.527   |        | Crippen Method |
| mcvol         | 298.080 | ml/mol | McGowan Method |
| rinpol        | 2878.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                             |
|-----------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C1169706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1169706&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>                                   |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                           |

## Legend

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

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