# Propanamide, N-phenyl-N-[1-(phenylmethyl)-4-piperidinyl]-

**Other names:** Propanamide, N-Phenyl-N-(1-benzyl-4-piperidinyl)-
Fentanyl methyl analog
Desmethylfentanyl
Benzylfentanyl
N-Benzylfentanyl
N-(1-benzylpiperidin-4-yl)-N-phenylpropionamide

**Inchi:** InChI=1S/C21H26N2O/c1-2-21(24)23(19-11-7-4-8-12-19)20-13-15-22(16-14-20)17-18-9-

**InchiKey:** POQDXIFVWVZVML-UHFFFAOYSA-N

**Formula:** C21H26N2O

**SMILES:** CCC(=O)N(c1ccccc1)C1CCN(Cc2ccccc2)CC1

**Mol. weight [g/mol]:** 322.44

**CAS:** 1474-02-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -4.77 | | Crippen Method |
| logp | 4.094 | | Crippen Method |
| mcvol | 269.900 | ml/mol | McGowan Method |
| rinpol | 2660.00 | | NIST Webbook |
| rinpol | 2690.00 | | NIST Webbook |
| rinpol | 2697.00 | | NIST Webbook |
| rinpol | 2697.00 | | NIST Webbook |
| rinpol | 2694.00 | | NIST Webbook |
| rinpol | 2693.00 | | NIST Webbook |
| rinpol | 2699.00 | | NIST Webbook |
| rinpol | 2682.00 | | NIST Webbook |
| rinpol | 2690.00 | | NIST Webbook |
| rinpol | 2699.00 | | NIST Webbook |
| rinpol | 2660.00 | | NIST Webbook |
| rinpol | 2692.00 | | NIST Webbook |

## Sources

**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1474028&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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