# Fentanyl, 4-N-octyl analogue

**Inchi:** InChI=1S/C22H36N2O/c1-3-5-6-7-8-12-17-23-18-15-21(16-19-23)24(22(25)4-2)20-13-10
**InchiKey:** CGZZCMMWVRVQCD-UHFFFAOYSA-N
**Formula:** C22H36N2O
**SMILES:** CCCCCCCCN1CCC(N(C(=O)CC)c2ccccc2)CC1
**Mol. weight [g/mol]:** 344.53

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| log10ws | -5.59 | | Crippen Method |
| logp | 5.255 | | Crippen Method |
| mcvol | 307.750 | ml/mol | McGowan Method |
| rinpol | 2651.00 | | NIST Webbook |
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| rinpol | 2671.00 | | NIST Webbook |
| rinpol | 2670.00 | | NIST Webbook |
| rinpol | 2676.00 | | NIST Webbook |
| rinpol | 2681.00 | | NIST Webbook |
| rinpol | 2684.00 | | NIST Webbook |
| rinpol | 2673.00 | | NIST Webbook |
| rinpol | 2676.00 | | NIST Webbook |
| rinpol | 2676.00 | | NIST Webbook |
| rinpol | 2670.00 | | NIST Webbook |
| rinpol | 2673.00 | | NIST Webbook |

## Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=R637559&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l
**Crippen Method:** https://www.chemeo.com/doc/models/crippen_log10ws
**McGowan Method:** http://link.springer.com/article/10.1007/BF02311772

# 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 |