

# Benproperine

**Inchi:** InChI=1S/C21H27NO/c1-18(22-14-8-3-9-15-22)17-23-21-13-7-6-12-20(21)16-19-10-4-2-5  
**InchiKey:** JTUQXGZRVLWBCR-UHFFFAOYSA-N  
**Formula:** C21H27NO  
**SMILES:** CC(COc1ccccc1Cc1ccccc1)N1CCCCC1  
**Mol. weight [g/mol]:** 309.45  
**CAS:** 2156-27-6

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.20   |        | Crippen Method |
| logp          | 4.531   |        | Crippen Method |
| mcvol         | 264.220 | ml/mol | McGowan Method |
| rinpola       | 2385.00 |        | NIST Webbook   |

## Sources

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2156276&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

## Legend

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

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