

# Methyldihydromorphine

|                             |                                                                                  |
|-----------------------------|----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C18H23NO3/c1-17(21)6-5-11-12-9-10-3-4-13(20)15-14(10)18(11,16(17)22-15) |
| <b>InchiKey:</b>            | NBKVWIJQJMEQLE-KDTAJPGPSA-N                                                      |
| <b>Formula:</b>             | C18H23NO3                                                                        |
| <b>SMILES:</b>              | CN1CCC23c4c5ccc(O)c4OC2C(C)(O)CCC3C1C5                                           |
| <b>Mol. weight [g/mol]:</b> | 301.38                                                                           |
| <b>CAS:</b>                 | 509-56-8                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.86   |        | Crippen Method |
| logp          | 1.812   |        | Crippen Method |
| mcvol         | 224.870 | ml/mol | McGowan Method |
| rinpol        | 2380.00 |        | NIST Webbook   |
| rinpol        | 2380.00 |        | NIST Webbook   |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C509568&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C509568&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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