

# Naloxone

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | (5«alpha»)-17-allyl-4,5-epoxy-3,14-dihydroxymorphinan-6-one hydrochloride        |
| Inchi:               | InChI=1S/C19H21NO4/c1-2-8-20-9-7-18-15-11-3-4-12(21)16(15)24-17(18)13(22)5-6-19( |
| InchiKey:            | UZHSEJADLWPNLE-OGLQFSJHSA-N                                                      |
| Formula:             | C19H21NO4                                                                        |
| SMILES:              | C=CCN1CCC23c4c5ccc(O)c4OC2C(=O)CCC3(O)C1C5                                       |
| Mol. weight [g/mol]: | 327.37                                                                           |
| CAS:                 | 357-08-4                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.65   |        | Crippen Method |
| logp          | 1.301   |        | Crippen Method |
| mcvol         | 236.230 | ml/mol | McGowan Method |
| rinpol        | 2608.00 |        | NIST Webbook   |
| rinpol        | 2644.00 |        | NIST Webbook   |
| rinpol        | 2644.00 |        | NIST Webbook   |
| rinpol        | 2655.00 |        | NIST Webbook   |
| rinpol        | 2640.00 |        | NIST Webbook   |
| rinpol        | 2608.00 |        | NIST Webbook   |
| rinpol        | 2640.00 |        | NIST Webbook   |
| rinpol        | 2608.00 |        | NIST Webbook   |
| rinpol        | 2644.00 |        | NIST Webbook   |
| rinpol        | 2655.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| 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>                         |
| 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=C357084&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C357084&amp;Units=SI</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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