

# Clemastine

|                      |                                                                                                                                                                                                                            |
|----------------------|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Pyrrolidine, 2-[2-[1-(4-chlorophenyl)-1-phenylethoxy]ethyl]-1-methyl-, [R-(R*,R*)]-(+)-(2R)-2-[2-[[[(R)-p-Chloro-«alpha»-methyl-«alpha»-phenylbenzyl]oxy]ethyl]-1-methylpyrrolidin-2-yl]-1-methylpyrrolidine<br>Meclastine |
| Inchi:               | InChI=1S/C21H26ClNO/c1-21(17-7-4-3-5-8-17,18-10-12-19(22)13-11-18)24-16-14-20-9-15                                                                                                                                         |
| InchiKey:            | YNNUSGIPVFPVBX-UHFFFAOYSA-N                                                                                                                                                                                                |
| Formula:             | C21H26ClNO                                                                                                                                                                                                                 |
| SMILES:              | CN1CCCC1CCOC(C)(c1ccccc1)c1ccc(Cl)cc1                                                                                                                                                                                      |
| Mol. weight [g/mol]: | 343.89                                                                                                                                                                                                                     |
| CAS:                 | 15686-51-8                                                                                                                                                                                                                 |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -5.44   |        | Crippen Method |
| logp          | 5.104   |        | Crippen Method |
| mcvol         | 276.460 | ml/mol | McGowan Method |
| rinpol        | 2430.00 |        | NIST Webbook   |
| rinpol        | 2415.00 |        | NIST Webbook   |
| rinpol        | 2420.00 |        | NIST Webbook   |
| rinpol        | 2420.00 |        | NIST Webbook   |
| rinpol        | 2446.00 |        | NIST Webbook   |
| rinpol        | 2420.00 |        | NIST Webbook   |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| 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=C15686518&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C15686518&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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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