

# Lupanine

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 7,14-Methano-4H,6H-dipyrido[1,2-a:1',2'-e][1,5]diazocin-4-one, dodecahydro-,<br>[7S-(7«alpha»,7a«beta»,14«alpha»,14a«alpha»)]-<br>(+)-Lupanine<br>2-Oxosparteine<br>Lupanin<br>d-Lupanine |
| <b>Inchi:</b>               | InChI=1S/C15H24N2O/c18-15-6-3-5-14-11-8-12(10-17(14)15)13-4-1-2-7-16(13)9-11/h11  |
| <b>InchiKey:</b>            | JYIJIVLEOETIQ-RQJABVFESA-N  |
| <b>Formula:</b>             | C15H24N2O   |
| <b>SMILES:</b>              | O=C1CCCC2C3CC(CN12)C1CCCCN1C3   |
| <b>Mol. weight [g/mol]:</b> | 248.36  |
| <b>CAS:</b>                 | 550-90-3  |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| log10ws       | -2.34   |        | Crippen Method |
| logp          | 1.872   |        | Crippen Method |
| mcvol         | 200.300 | ml/mol | McGowan Method |
| rinpol        | 2159.00 |        | NIST Webbook   |
| rinpol        | 2165.00 |        | NIST Webbook   |
| rinpol        | 2178.00 |        | NIST Webbook   |
| rinpol        | 2185.00 |        | NIST Webbook   |
| rinpol        | 2193.00 |        | NIST Webbook   |
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| rinpol | 2160.00 | NIST Webbook |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C550903&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C550903&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</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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