

# 5«beta»-Pregnane-3,20-dione, bis(O-methyloxime)

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | 5«beta»-Pregnan-3,20-dione, MO                                                   |
| Inchi:               | InChI=1S/C23H38N2O2/c1-15(24-26-4)19-8-9-20-18-7-6-16-14-17(25-27-5)10-12-22(16, |
| InchiKey:            | BRBZYVRSVCPKEU-BJEAQBELSA-N                                                      |
| Formula:             | C23H38N2O2                                                                       |
| SMILES:              | CON=C1CCC2(C)C(CCC3C2CCC2(C)C(C(C)=NOC)CCC32)C1                                  |
| Mol. weight [g/mol]: | 374.56                                                                           |
| CAS:                 | 3091-37-0                                                                        |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | -439.17 | kJ/mol | Joback Method  |
| hvap          | 76.43   | kJ/mol | Joback Method  |
| log10ws       | -5.82   |        | Crippen Method |
| logp          | 5.670   |        | Crippen Method |
| mcvol         | 314.590 | ml/mol | McGowan Method |
| pc            | 1073.57 | kPa    | Joback Method  |
| rinpol        | 2740.00 |        | NIST Webbook   |
| tb            | 960.98  | K      | Joback Method  |
| tc            | 1206.29 | K      | Joback Method  |

## 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>                           |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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=C3091370&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3091370&amp;Units=SI</a> |

## Legend

hf: Enthalpy of formation at standard conditions

|                                       |                                                 |
|---------------------------------------|-------------------------------------------------|
| <b>h<sub>vap</sub>:</b>               | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>w<sub>s</sub>:</b> | Log10 of Water solubility in mol/l              |
| <b>log<sub>p</sub>:</b>               | Octanol/Water partition coefficient             |
| <b>mc<sub>vol</sub>:</b>              | McGowan's characteristic volume                 |
| <b>p<sub>c</sub>:</b>                 | Critical Pressure                               |
| <b>ri<sub>npol</sub>:</b>             | Non-polar retention indices                     |
| <b>t<sub>b</sub>:</b>                 | Normal Boiling Point Temperature                |
| <b>t<sub>c</sub>:</b>                 | Critical Temperature                            |

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