

# Laurenene

|                             |                                                                                   |
|-----------------------------|-----------------------------------------------------------------------------------|
| <b>Inchi:</b>               | InChI=1S/C20H32/c1-14-7-6-10-18(4)12-9-16-17(2,3)13-19(5)11-8-15(14)20(16,18)19/h |
| <b>InchiKey:</b>            | TYDFDHZTDWVUJF-ULKVZQIESA-N                                                       |
| <b>Formula:</b>             | C20H32                                                                            |
| <b>SMILES:</b>              | CC1CCCC2(C)CCC3C(C)(C)CC4(C)CC=C1C324                                             |
| <b>Mol. weight [g/mol]:</b> | 272.47                                                                            |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 307.17  | kJ/mol               | Joback Method  |
| hf            | -116.82 | kJ/mol               | Joback Method  |
| hfus          | 11.58   | kJ/mol               | Joback Method  |
| hvap          | 56.01   | kJ/mol               | Joback Method  |
| log10ws       | -6.18   |                      | Crippen Method |
| logp          | 5.975   |                      | Crippen Method |
| mcvol         | 244.920 | ml/mol               | McGowan Method |
| pc            | 1724.59 | kPa                  | Joback Method  |
| rinpol        | 1935.00 |                      | NIST Webbook   |
| rinpol        | 1872.00 |                      | NIST Webbook   |
| tb            | 692.53  | K                    | Joback Method  |
| tc            | 936.67  | K                    | Joback Method  |
| tf            | 476.76  | K                    | Joback Method  |
| vc            | 0.935   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 762.21 | J/mol×K | 692.53          | Joback Method |
| cpg           | 788.76 | J/mol×K | 733.22          | Joback Method |
| cpg           | 814.91 | J/mol×K | 773.91          | Joback Method |
| cpg           | 841.35 | J/mol×K | 814.60          | Joback Method |
| cpg           | 868.72 | J/mol×K | 855.29          | Joback Method |
| cpg           | 897.71 | J/mol×K | 895.98          | Joback Method |
| cpg           | 928.97 | J/mol×K | 936.67          | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R201546&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R201546&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>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvpap:</b>   | Enthalpy of vaporization at standard conditions |
| <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>pc:</b>      | Critical Pressure                               |
| <b>rinppl:</b>  | Non-polar retention indices                     |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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