

# Ninhydrin

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 1H-Indene-1,3(2H)-dione, 2,2-dihydroxy-1,3-Indandione, 2,2-dihydroxy-Ningidrin<br>Ninhydrin hydrate<br>Triketohydrindene hydrate<br>2,2-Dihydroxy-1,3-indandione<br>2,2-Dihydroxy-1H-indene-1,3(2H)-dione<br>1,2,3-Indantrione, 2-hydrate<br>1,2,3-Indantrione monohydrate<br>1H-Indene-1,2,3-trione, 2-hydrate<br>indan-1,2,3-trione |
| <b>Inchi:</b>               | InChI=1S/C9H6O4/c10-7-5-3-1-2-4-6(5)8(11)9(7,12)13/h1-4,12-13H  |
| <b>InchiKey:</b>            | FEMOMIGRRWSMCU-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C9H6O4  |
| <b>SMILES:</b>              | <chem>O=C1c2ccccc2C(=O)C1(O)O</chem>  |
| <b>Mol. weight [g/mol]:</b> | 178.14  |
| <b>CAS:</b>                 | 485-47-2  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -335.88 | kJ/mol  | Joback Method  |
| hf            | -495.85 | kJ/mol  | Joback Method  |
| hfus          | 11.75   | kJ/mol  | Joback Method  |
| hvap          | 79.18   | kJ/mol  | Joback Method  |
| log10ws       | -1.40   |         | Crippen Method |
| logp          | -0.254  |         | Crippen Method |
| mcvol         | 117.930 | ml/mol  | McGowan Method |
| pc            | 5594.19 | kPa     | Joback Method  |
| tb            | 763.96  | K       | Joback Method  |
| tc            | 989.71  | K       | Joback Method  |
| tf            | 530.05  | K       | Joback Method  |
| vc            | 0.439   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 328.92 | J/mol×K | 763.96          | Joback Method |
| cpg           | 337.96 | J/mol×K | 801.58          | Joback Method |
| cpg           | 346.81 | J/mol×K | 839.21          | Joback Method |
| cpg           | 355.57 | J/mol×K | 876.83          | Joback Method |
| cpg           | 364.33 | J/mol×K | 914.46          | Joback Method |
| cpg           | 373.19 | J/mol×K | 952.08          | Joback Method |
| cpg           | 382.23 | J/mol×K | 989.71          | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C485472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C485472&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>hvap:</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>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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