

# neral dimethyl acetal

**Inchi:** InChI=1S/C12H22O2/c1-10(2)7-6-8-11(3)9-12(13-4)14-5/h7,9,12H,6,8H2,1-5H3/b11-9-  
**InchiKey:** ZSKAJFSSXURRGL-LUAWRHEFSA-N  
**Formula:** C12H22O2  
**SMILES:** COC(C=C(C)CCC=C(C)C)OC  
**Mol. weight [g/mol]:** 198.30

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -18.94  | kJ/mol  | Joback Method  |
| hf            | -345.87 | kJ/mol  | Joback Method  |
| hfus          | 23.47   | kJ/mol  | Joback Method  |
| hvap          | 46.81   | kJ/mol  | Joback Method  |
| log10ws       | -3.33   |         | Crippen Method |
| logp          | 3.298   |         | Crippen Method |
| mcvol         | 183.080 | ml/mol  | McGowan Method |
| pc            | 1920.30 | kPa     | Joback Method  |
| rinpol        | 1300.40 |         | NIST Webbook   |
| tb            | 526.44  | K       | Joback Method  |
| tc            | 710.27  | K       | Joback Method  |
| tf            | 216.38  | K       | Joback Method  |
| vc            | 0.700   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 429.35 | J/mol×K | 526.44          | Joback Method |
| cpg           | 445.83 | J/mol×K | 557.08          | Joback Method |
| cpg           | 461.59 | J/mol×K | 587.72          | Joback Method |
| cpg           | 476.65 | J/mol×K | 618.36          | Joback Method |
| cpg           | 491.03 | J/mol×K | 648.99          | Joback Method |
| cpg           | 504.77 | J/mol×K | 679.63          | Joback Method |
| cpg           | 517.86 | J/mol×K | 710.27          | 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=R185885&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R185885&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>rinpol:</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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