

# Acetoxyacetamide, N,N-dinonyl-

**Inchi:** InChI=1S/C22H43NO3/c1-4-6-8-10-12-14-16-18-23(22(25)20-26-21(3)24)19-17-15-13-11  
**InchiKey:** SJJYQPVVQQCLJG-UHFFFAOYSA-N  
**Formula:** C22H43NO3  
**SMILES:** CCCCCCCCCN(CCCCCCCC)C(=O)COC(C)=O  
**Mol. weight [g/mol]:** 369.58

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -117.70 | kJ/mol               | Joback Method  |
| hf            | -787.26 | kJ/mol               | Joback Method  |
| hfus          | 60.14   | kJ/mol               | Joback Method  |
| hvap          | 82.51   | kJ/mol               | Joback Method  |
| log10ws       | -6.24   |                      | Crippen Method |
| logp          | 5.879   |                      | Crippen Method |
| mcvol         | 339.830 | ml/mol               | McGowan Method |
| pc            | 962.67  | kPa                  | Joback Method  |
| rinpol        | 2583.00 |                      | NIST Webbook   |
| rinpol        | 2583.00 |                      | NIST Webbook   |
| tb            | 845.36  | K                    | Joback Method  |
| tc            | 1035.07 | K                    | Joback Method  |
| tf            | 492.26  | K                    | Joback Method  |
| vc            | 1.315   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1103.73 | J/mol×K | 845.36          | Joback Method |
| cpg           | 1123.29 | J/mol×K | 876.98          | Joback Method |
| cpg           | 1141.71 | J/mol×K | 908.60          | Joback Method |
| cpg           | 1159.02 | J/mol×K | 940.21          | Joback Method |
| cpg           | 1175.28 | J/mol×K | 971.83          | Joback Method |
| cpg           | 1190.51 | J/mol×K | 1003.45         | Joback Method |
| cpg           | 1204.77 | J/mol×K | 1035.07         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <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>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308299&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308299&amp;Units=SI</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>hvp:</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>rinp:</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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