

# Malonic acid, dimethylaminomethylene-, diethyl ester

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | Propanedioic acid, [(dimethylamino)methylene]-, diethyl ester           |
| <b>Inchi:</b>               | InChI=1S/C10H17NO4/c1-5-14-9(12)8(7-11(3)4)10(13)15-6-2/h7H,5-6H2,1-4H3 |
| <b>InchiKey:</b>            | XNSXXTKUKYWLAH-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C10H17NO4   |
| <b>SMILES:</b>              | CCOC(=O)C(=CN(C)C)C(=O)OCC  |
| <b>Mol. weight [g/mol]:</b> | 215.25  |
| <b>CAS:</b>                 | 18856-68-3  |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -252.07 | kJ/mol               | Joback Method  |
| hf            | -564.37 | kJ/mol               | Joback Method  |
| hfus          | 29.14   | kJ/mol               | Joback Method  |
| hvap          | 58.25   | kJ/mol               | Joback Method  |
| log10ws       | -0.65   |                      | Crippen Method |
| logp          | 0.558   |                      | Crippen Method |
| mcvol         | 172.320 | ml/mol               | McGowan Method |
| pc            | 2424.27 | kPa                  | Joback Method  |
| tb            | 597.26  | K                    | Joback Method  |
| tc            | 785.31  | K                    | Joback Method  |
| tf            | 360.21  | K                    | Joback Method  |
| vc            | 0.642   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 431.91 | J/mol×K | 597.26          | Joback Method |
| cpg           | 445.30 | J/mol×K | 628.60          | Joback Method |
| cpg           | 458.04 | J/mol×K | 659.94          | Joback Method |
| cpg           | 470.13 | J/mol×K | 691.28          | Joback Method |
| cpg           | 481.59 | J/mol×K | 722.63          | Joback Method |
| cpg           | 492.43 | J/mol×K | 753.97          | Joback Method |
| cpg           | 502.66 | J/mol×K | 785.31          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C18856683&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C18856683&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>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>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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