

# Glycinonitrile, n-methylene-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 2-(methyleneamino)acetonitrile<br>methyleneaminoacetonitrile |
| <b>Inchi:</b>               | InChI=1S/C3H4N2/c1-5-3-2-4/h1,3H2                            |
| <b>InchiKey:</b>            | GFZMFCVDDFHSJK-UHFFFAOYSA-N                                  |
| <b>Formula:</b>             | C3H4N2   |
| <b>SMILES:</b>              | C=NCC#N  |
| <b>Mol. weight [g/mol]:</b> | 68.08  |
| <b>CAS:</b>                 | 109-82-0   |

## Physical Properties

| Property code | Value   | Unit   | Source  |
|---------------|---------|--------|---|
| hf            | 150.06  | kJ/mol | Joback Method   |
| hvap          | 35.44   | kJ/mol | Joback Method   |
| ie            | 10.20   | eV     | NIST Webbook  |
| ie            | 10.60   | eV     | NIST Webbook  |
| log10ws       | -0.11   |        | Crippen Method  |
| logp          | 0.211   |        | Crippen Method  |
| mvol          | 60.190  | ml/mol | McGowan Method  |
| pc            | 3690.97 | kPa    | Joback Method   |
| tb            | 439.32  | K      | Joback Method   |
| tc            | 651.30  | K      | Joback Method   |
| tt            | 402.15  | K      | Measurement and correlation of solubility of methyleneaminoacetonitrile in pure and binary solvents and thermodynamic properties of solution                  |
| tt            | 400.19  | K      | Solubility behaviour and thermodynamic analysis of methyleneaminoacetonitrile in binary (ethanol + water, ethanol + 2-propanol, ethanol + n-butanol) solvents |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C109820&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Measurement and correlation of solubility of propylene carbonate and methyl methacrylate in pure and binary solvents and thermodynamic analysis of Joback's method for the prediction of dynamic properties of nitrile in binary systems (ethanol + water, ethanol + 2-propanol, ethanol + n-butanol) solvents:** <https://www.doi.org/10.1016/j.jct.2019.01.015>  
<https://www.doi.org/10.1016/j.jct.2019.06.009>  
[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## Legend

**hf:** Enthalpy of formation at standard conditions  
**hvap:** Enthalpy of vaporization at standard conditions  
**ie:** Ionization energy  
**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume  
**pc:** Critical Pressure  
**tb:** Normal Boiling Point Temperature  
**tc:** Critical Temperature  
**tt:** Triple Point Temperature

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