

# 5-Hexynenitrile

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-Cyano-1-pentyne<br>5-cyanopent-1-yne  |
| <b>Inchi:</b>               | InChI=1S/C6H7N/c1-2-3-4-5-6-7/h1H,3-5H2 |
| <b>InchiKey:</b>            | JZYKFLLRVPPISG-UHFFFAOYSA-N             |
| <b>Formula:</b>             | C6H7N                                   |
| <b>SMILES:</b>              | C#CCCCC#N                               |
| <b>Mol. weight [g/mol]:</b> | 93.13                                   |
| <b>CAS:</b>                 | 14918-21-9                              |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 355.89  | kJ/mol               | Joback Method  |
| hf            | 289.61  | kJ/mol               | Joback Method  |
| hfus          | 15.78   | kJ/mol               | Joback Method  |
| hvap          | 39.29   | kJ/mol               | Joback Method  |
| log10ws       | -2.00   |                      | Crippen Method |
| logp          | 1.313   |                      | Crippen Method |
| mvol          | 88.180  | ml/mol               | McGowan Method |
| pc            | 3581.35 | kPa                  | Joback Method  |
| tb            | 428.88  | K                    | Joback Method  |
| tc            | 631.83  | K                    | Joback Method  |
| tf            | 269.34  | K                    | Joback Method  |
| vc            | 0.359   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 162.56 | J/mol×K | 428.88          | Joback Method |
| cpg           | 169.98 | J/mol×K | 462.70          | Joback Method |
| cpg           | 177.02 | J/mol×K | 496.53          | Joback Method |
| cpg           | 183.68 | J/mol×K | 530.35          | Joback Method |
| cpg           | 190.01 | J/mol×K | 564.18          | Joback Method |
| cpg           | 195.99 | J/mol×K | 598.00          | Joback Method |
| cpg           | 201.67 | J/mol×K | 631.83          | Joback Method |

# Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 389.00 ± 1.00 | K    | 14.90          | NIST Webbook |

## 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=C14918219&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14918219&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>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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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