

# 4-Nonene, 5-nitro-

|                             |   |
|-----------------------------|---|
| <b>Other names:</b>         | 5-Nitro-4-nonene  |
| <b>Inchi:</b>               | InChI=1S/C9H17NO2/c1-3-5-7-9(10(11)12)8-6-4-2/h7H,3-6,8H2,1-2H3/b9-7+ |
| <b>InchiKey:</b>            | QTNRZJBKFAASKI-VQHVLOKHSA-N   |
| <b>Formula:</b>             | C9H17NO2  |
| <b>SMILES:</b>              | CCCC=C(CCCC)[N+](=O)[O-]  |
| <b>Mol. weight [g/mol]:</b> | 171.24  |
| <b>CAS:</b>                 | 6065-01-6   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 132.12  | kJ/mol               | Joback Method  |
| hf            | -132.42 | kJ/mol               | Joback Method  |
| hfus          | 29.32   | kJ/mol               | Joback Method  |
| hvap          | 52.26   | kJ/mol               | Joback Method  |
| log10ws       | -4.02   |                      | Crippen Method |
| logp          | 3.137   |                      | Crippen Method |
| mcvol         | 150.790 | ml/mol               | McGowan Method |
| pc            | 2467.81 | kPa                  | Joback Method  |
| tb            | 561.20  | K                    | Joback Method  |
| tc            | 766.84  | K                    | Joback Method  |
| tf            | 315.76  | K                    | Joback Method  |
| vc            | 0.603   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 365.87 | J/mol×K | 561.20          | Joback Method |
| cpg           | 380.08 | J/mol×K | 595.47          | Joback Method |
| cpg           | 393.50 | J/mol×K | 629.75          | Joback Method |
| cpg           | 406.17 | J/mol×K | 664.02          | Joback Method |
| cpg           | 418.13 | J/mol×K | 698.29          | Joback Method |
| cpg           | 429.42 | J/mol×K | 732.57          | Joback Method |
| cpg           | 440.09 | J/mol×K | 766.84          | 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=C6065016&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6065016&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>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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