

# 2-Propen-1-amine, N-ethyl-

|                      |                                                |
|----------------------|------------------------------------------------|
| Other names:         | Allylethylamine<br>N-ethylallylamine           |
| Inchi:               | InChI=1S/C5H11N/c1-3-5-6-4-2/h3,6H,1,4-5H2,2H3 |
| InchiKey:            | PUUULGNNRPBVBA-UHFFFAOYSA-N                    |
| Formula:             | C5H11N                                         |
| SMILES:              | C=CCNCC                                        |
| Mol. weight [g/mol]: | 85.15                                          |
| CAS:                 | 2424-02-4                                      |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 168.45  | kJ/mol  | Joback Method  |
| hf            | 32.37   | kJ/mol  | Joback Method  |
| hfus          | 12.52   | kJ/mol  | Joback Method  |
| hvap          | 32.49   | kJ/mol  | Joback Method  |
| log10ws       | -0.96   |         | Crippen Method |
| logp          | 0.782   |         | Crippen Method |
| mcvol         | 86.990  | ml/mol  | McGowan Method |
| pc            | 3704.46 | kPa     | Joback Method  |
| rinpol        | 640.00  |         | NIST Webbook   |
| rinpol        | 640.00  |         | NIST Webbook   |
| tb            | 360.65  | K       | Joback Method  |
| tc            | 534.49  | K       | Joback Method  |
| tf            | 197.01  | K       | Joback Method  |
| vc            | 0.332   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 149.09 | J/mol×K | 360.65          | Joback Method |
| cpg           | 158.57 | J/mol×K | 389.62          | Joback Method |
| cpg           | 167.67 | J/mol×K | 418.60          | Joback Method |
| cpg           | 176.39 | J/mol×K | 447.57          | Joback Method |
| cpg           | 184.75 | J/mol×K | 476.54          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 192.75 | J/mol×K | 505.52 | Joback Method |
| cpg | 200.41 | J/mol×K | 534.49 | Joback Method |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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>                                   |
| <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=C2424024&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2424024&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>rinpol:</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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