

# 2-Pentanamine

|                      |                                                                                                                                                                                                                                                                                                                              |
|----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | (±)-1-methylbutylamine<br>( $\hat{A}$ ±)-1-methylbutylamine<br>1-Methyl-n-butylamine<br>1-Methylbutylamine<br>2-Aminopentane<br>2-Amylamine<br>2-Pentanamine, (.+/-.)-<br>2-Pentylamine<br>Butylamine, 1-methyl-<br>DL-2-Aminopentane<br>NSC 6367<br>sec-Amylamine<br>«alpha»-Methylbutylamine<br>Â«alphaÂ»-Methylbutylamine |
| Inchi:               | InChI=1S/C5H13N/c1-3-4-5(2)6/h5H,3-4,6H2,1-2H3                                                                                                                                                                                                                                                                               |
| InchiKey:            | IGEIPFLJVCPEKU-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                  |
| Formula:             | C5H13N                                                                                                                                                                                                                                                                                                                       |
| SMILES:              | CCCC(C)N                                                                                                                                                                                                                                                                                                                     |
| Mol. weight [g/mol]: | 87.16                                                                                                                                                                                                                                                                                                                        |
| CAS:                 | 63493-28-7                                                                                                                                                                                                                                                                                                                   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 55.23   | kJ/mol  | Joback Method  |
| hf            | -118.02 | kJ/mol  | Joback Method  |
| hfus          | 10.38   | kJ/mol  | Joback Method  |
| hvap          | 36.98   | kJ/mol  | Joback Method  |
| log10ws       | -1.46   |         | Crippen Method |
| logp          | 1.134   |         | Crippen Method |
| mcvol         | 91.290  | ml/mol  | McGowan Method |
| pc            | 3749.97 | kPa     | Joback Method  |
| tb            | 385.89  | K       | Joback Method  |
| tc            | 571.20  | K       | Joback Method  |
| tf            | 214.37  | K       | Joback Method  |
| vc            | 0.339   | m3/kmol | Joback Method  |

# Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 173.57 | J/mol×K | 385.89          | Joback Method |
| cpg           | 184.03 | J/mol×K | 416.77          | Joback Method |
| cpg           | 194.06 | J/mol×K | 447.66          | Joback Method |
| cpg           | 203.68 | J/mol×K | 478.54          | Joback Method |
| cpg           | 212.89 | J/mol×K | 509.43          | Joback Method |
| cpg           | 221.72 | J/mol×K | 540.31          | Joback Method |
| cpg           | 230.17 | J/mol×K | 571.20          | Joback Method |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.40749e+01                   |
| Coeff. B                    | -2.65083e+03                  |
| Coeff. C                    | -8.38820e+01                  |
| Temperature range (K), min. | 276.15                        |
| Temperature range (K), max. | 386.37                        |

## Sources

|                                      |                                                                                                                                                                                         |
|--------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method:                      | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                                                                       |
| Joback Method:                       | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                                                                   |
| McGowan Method:                      | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                                                                   |
| NIST Webbook:                        | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C63493287&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C63493287&amp;Units=SI</a>                                           |
| The Yaws Handbook of Vapor Pressure: | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| Crippen Method:                      | <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>pvap:</b>    | Vapor 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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