

# P-sec-amylaniline

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C11H17N/c1-3-4-9(2)10-5-7-11(12)8-6-10/h5-9H,3-4,12H2,1-2H3 |
| <b>InchiKey:</b>            | AKSSDFIINGVZJQ-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C11H17N  |
| <b>SMILES:</b>              | CCCC(C)c1ccc(N)cc1   |
| <b>Mol. weight [g/mol]:</b> | 163.26   |
| <b>CAS:</b>                 | 30273-14-4   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 208.53  | kJ/mol  | Joback Method  |
| hf            | -16.80  | kJ/mol  | Joback Method  |
| hfus          | 19.57   | kJ/mol  | Joback Method  |
| hvap          | 53.27   | kJ/mol  | Joback Method  |
| log10ws       | -3.13   |         | Crippen Method |
| logp          | 3.172   |         | Crippen Method |
| mcvol         | 152.070 | ml/mol  | McGowan Method |
| pc            | 2790.61 | kPa     | Joback Method  |
| tb            | 554.83  | K       | Joback Method  |
| tc            | 772.79  | K       | Joback Method  |
| tf            | 320.93  | K       | Joback Method  |
| vc            | 0.567   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 362.99 | J/molxK | 554.83          | Joback Method |
| cpg           | 378.84 | J/molxK | 591.16          | Joback Method |
| cpg           | 393.76 | J/molxK | 627.48          | Joback Method |
| cpg           | 407.78 | J/molxK | 663.81          | Joback Method |
| cpg           | 420.95 | J/molxK | 700.14          | Joback Method |
| cpg           | 433.29 | J/molxK | 736.46          | Joback Method |
| cpg           | 444.85 | J/molxK | 772.79          | 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=C30273144&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C30273144&amp;Units=SI</a> |
| <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>                                     |

# 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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