

# o-(o-Tolyloxy)aniline

|                      |                                                                                                                                |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | 2-Amino-2'-methyldiphenyl ether<br>Benzenamine, 2-(2-methylphenoxy)-<br>Aniline, 2-(o-tolyloxy)-<br>2-(2-methylphenoxy)aniline |
| Inchi:               | InChI=1S/C13H13NO/c1-10-6-2-4-8-12(10)15-13-9-5-3-7-11(13)14/h2-9H,14H2,1H3                                                    |
| InchiKey:            | JYJPXACGURQSCB-UHFFFAOYSA-N                                                                                                    |
| Formula:             | C13H13NO                                                                                                                       |
| SMILES:              | Cc1ccccc1Oc1ccccc1N                                                                                                            |
| Mol. weight [g/mol]: | 199.25                                                                                                                         |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | 26.42   | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 23.12   | kJ/mol | Joback Method      |
| hvap          | 80.30   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 7.33    | eV     | Cheméo Relay (1.0) |
| log10ws       | -3.13   |        | Cheméo Relay (1.0) |
| logp          | 3.370   |        | Crippen Method     |
| mcvol         | 162.360 | ml/mol | McGowan Method     |
| pc            | 3107.10 | kPa    | Joback Method      |
| tb            | 578.78  | K      | Cheméo Relay (1.0) |
| tc            | 862.55  | K      | Cheméo Relay (1.0) |
| tf            | 331.35  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 408.08 | J/mol×K | 655.11          | Joback Method |
| cpg           | 423.20 | J/mol×K | 696.72          | Joback Method |
| cpg           | 437.17 | J/mol×K | 738.32          | Joback Method |
| cpg           | 450.03 | J/mol×K | 779.93          | Joback Method |
| cpg           | 461.82 | J/mol×K | 821.53          | Joback Method |
| cpg           | 472.59 | J/mol×K | 863.14          | Joback Method |
| cpg           | 482.38 | J/mol×K | 904.74          | 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>Cheméo Relay (1.0):</b>       |                                                                                                                                             |
| <b>Cheméo Relay (1.0, beta):</b> |                                                                                                                                             |
| <b>NIST Webbook:</b>             | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3840184&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3840184&amp;Units=SI</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>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>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>ie:</b>      | Ionization energy                               |
| <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                   |

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