

# N,N-DIETHYL-4-TOLUAMIDE

|                      |                                                                                           |
|----------------------|-------------------------------------------------------------------------------------------|
| Other names:         | p-DETA<br>p-Toluamide, N,N-diethyl-<br>N,N-Diethyl-p-toluamide<br>N,N-Diethyl-4-toluamide |
| Inchi:               | InChI=1S/C12H17NO/c1-4-13(5-2)12(14)11-8-6-10(3)7-9-11/h6-9H,4-5H2,1-3H3                  |
| InchiKey:            | PUZORFQMRDHKBT-UHFFFAOYSA-N                                                               |
| Formula:             | C12H17NO                                                                                  |
| SMILES:              | CCN(CC)C(=O)c1ccc(C)cc1                                                                   |
| Mol. weight [g/mol]: | 191.27                                                                                    |

## Physical Properties

| Property code | Value   | Unit   | Source             |
|---------------|---------|--------|--------------------|
| hf            | -186.66 | kJ/mol | Cheméo Relay (1.0) |
| hfus          | 25.11   | kJ/mol | Joback Method      |
| hvap          | 68.47   | kJ/mol | Cheméo Relay (1.0) |
| ie            | 8.05    | eV     | Cheméo Relay (1.0) |
| log10ws       | -2.75   |        | Cheméo Relay (1.0) |
| logp          | 2.477   |        | Crippen Method     |
| mcvol         | 167.730 | ml/mol | McGowan Method     |
| tb            | 568.31  | K      | Cheméo Relay (1.0) |
| tc            | 751.98  | K      | Cheméo Relay (1.0) |
| tf            | 309.50  | K      | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 404.24 | J/mol×K | 571.93          | Joback Method |
| cpg           | 420.02 | J/mol×K | 606.31          | Joback Method |
| cpg           | 434.87 | J/mol×K | 640.68          | Joback Method |
| cpg           | 448.82 | J/mol×K | 675.06          | Joback Method |
| cpg           | 461.92 | J/mol×K | 709.43          | Joback Method |
| cpg           | 474.20 | J/mol×K | 743.81          | Joback Method |
| cpg           | 485.70 | J/mol×K | 778.19          | Joback Method |

# Sources

**Cheméo Relay (1.0, beta):**

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C2728054&Units=SI>

**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>

**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

**Cheméo Relay (1.0):**

## 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>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |

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