

# Diethyl tert-butylamine

|                      |                                                 |
|----------------------|-------------------------------------------------|
| Other names:         | 2-Propanamine, 2-methyl, N,N-diethyl            |
| Inchi:               | InChI=1S/C8H19N/c1-6-9(7-2)8(3,4)5/h6-7H2,1-5H3 |
| InchiKey:            | UPNQFYMXRSHQBY-UHFFFAOYSA-N                     |
| Formula:             | C8H19N                                          |
| SMILES:              | CCN(CC)C(C)(C)C                                 |
| Mol. weight [g/mol]: | 129.24                                          |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | 130.10  | kJ/mol  | Joback Method  |
| hf            | -149.67 | kJ/mol  | Joback Method  |
| hfus          | 12.08   | kJ/mol  | Joback Method  |
| hvap          | 34.15   | kJ/mol  | Joback Method  |
| log10ws       | -1.85   |         | Crippen Method |
| logp          | 2.127   |         | Crippen Method |
| mcvol         | 133.560 | ml/mol  | McGowan Method |
| pc            | 2579.34 | kPa     | Joback Method  |
| rinpol        | 814.00  |         | NIST Webbook   |
| tb            | 391.65  | K       | Joback Method  |
| tc            | 564.43  | K       | Joback Method  |
| tf            | 214.81  | K       | Joback Method  |
| vc            | 0.490   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 262.31 | J/mol×K | 391.65          | Joback Method |
| cpg           | 277.98 | J/mol×K | 420.45          | Joback Method |
| cpg           | 292.90 | J/mol×K | 449.24          | Joback Method |
| cpg           | 307.10 | J/mol×K | 478.04          | Joback Method |
| cpg           | 320.61 | J/mol×K | 506.84          | Joback Method |
| cpg           | 333.45 | J/mol×K | 535.63          | Joback Method |
| cpg           | 345.65 | J/mol×K | 564.43          | 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=R12903&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R12903&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>rlnpol:</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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