

# 2-(tert-Butylamino)ethanol

|                      |                                                                                                                                                                                                                                |
|----------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | N-t-Butylethanolamine<br>tert-Butylethanolamine<br>N-tert-Butylethanolamine<br>Ethanol, 2-[(1,1-dimethylethyl)amino]-<br>«beta»-tert-Butylaminoethanol<br>tert-Butylaminoethanol<br>Ethanol, 2-(tert-butylamino)-<br>NSC 78430 |
| Inchi:               | InChI=1S/C6H15NO/c1-6(2,3)7-4-5-8/h7-8H,4-5H2,1-3H3                                                                                                                                                                            |
| InchiKey:            | IUXYVKZUDNLISR-UHFFFAOYSA-N                                                                                                                                                                                                    |
| Formula:             | C6H15NO                                                                                                                                                                                                                        |
| SMILES:              | CC(C)(C)NCCO                                                                                                                                                                                                                   |
| Mol. weight [g/mol]: | 117.19                                                                                                                                                                                                                         |
| CAS:                 | 4620-70-6                                                                                                                                                                                                                      |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -44.95  | kJ/mol  | Joback Method  |
| hf            | -274.68 | kJ/mol  | Joback Method  |
| hfus          | 13.07   | kJ/mol  | Joback Method  |
| hvap          | 50.77   | kJ/mol  | Joback Method  |
| log10ws       | -0.90   |         | Crippen Method |
| logp          | 0.367   |         | Crippen Method |
| mcvol         | 111.250 | ml/mol  | McGowan Method |
| pc            | 3585.64 | kPa     | Joback Method  |
| tb            | 449.70  | K       | NIST Webbook   |
| tc            | 650.46  | K       | Joback Method  |
| tf            | 273.28  | K       | Joback Method  |
| vc            | 0.414   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 253.51 | J/mol×K | 475.80          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 264.48 | J/mol×K | 504.91 | Joback Method |
| cpg | 274.92 | J/mol×K | 534.02 | Joback Method |
| cpg | 284.82 | J/mol×K | 563.13 | Joback Method |
| cpg | 294.23 | J/mol×K | 592.24 | Joback Method |
| cpg | 303.15 | J/mol×K | 621.35 | Joback Method |
| cpg | 311.62 | J/mol×K | 650.46 | Joback Method |

## Pressure Dependent Properties

| Property code | Value         | Unit | Pressure [kPa] | Source       |
|---------------|---------------|------|----------------|--------------|
| tbrp          | 364.20        | K    | 3.30           | NIST Webbook |
| tbrp          | 364.00 ± 1.00 | K    | 3.30           | NIST Webbook |

## Sources

|                        |                                                                                                                                             |
|------------------------|---------------------------------------------------------------------------------------------------------------------------------------------|
| <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=C4620706&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4620706&amp;Units=SI</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>                                   |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>tbrp:</b>    | Boiling point at reduced pressure               |
| <b>tc:</b>      | Critical Temperature                            |

**tf:** Normal melting (fusion) point  
**vc:** Critical Volume

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