

# Isobutenyl amine, n,n-dimethyl-

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | 1-Propen-1-amine, N,N,2-trimethyl-       |
| <b>Inchi:</b>               | InChI=1S/C6H13N/c1-6(2)5-7(3)4/h5H,1-4H3 |
| <b>InchiKey:</b>            | IHSJXWLJYTXOCL-UHFFFAOYSA-N              |
| <b>Formula:</b>             | C6H13N                                   |
| <b>SMILES:</b>              | CC(C)=CN(C)C                             |
| <b>Mol. weight [g/mol]:</b> | 99.17                                    |
| <b>CAS:</b>                 | 6906-32-7                                |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| affp          | 967.00  | kJ/mol               | NIST Webbook   |
| basg          | 934.50  | kJ/mol               | NIST Webbook   |
| gf            | 182.09  | kJ/mol               | Joback Method  |
| hf            | 7.79    | kJ/mol               | Joback Method  |
| hfus          | 13.21   | kJ/mol               | Joback Method  |
| hvap          | 31.03   | kJ/mol               | Joback Method  |
| ie            | 8.15    | eV                   | NIST Webbook   |
| log10ws       | -1.25   |                      | Crippen Method |
| logp          | 1.472   |                      | Crippen Method |
| mcvol         | 101.080 | ml/mol               | McGowan Method |
| pc            | 3306.75 | kPa                  | Joback Method  |
| tb            | 353.16  | K                    | Joback Method  |
| tc            | 527.98  | K                    | Joback Method  |
| tf            | 170.81  | K                    | Joback Method  |
| vc            | 0.370   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 170.27 | J/mol×K | 353.16          | Joback Method |
| cpg           | 182.17 | J/mol×K | 382.30          | Joback Method |
| cpg           | 193.51 | J/mol×K | 411.43          | Joback Method |
| cpg           | 204.31 | J/mol×K | 440.57          | Joback Method |
| cpg           | 214.58 | J/mol×K | 469.71          | Joback Method |

|     |        |         |        |               |
|-----|--------|---------|--------|---------------|
| cpg | 224.36 | J/mol×K | 498.84 | Joback Method |
| cpg | 233.65 | J/mol×K | 527.98 | 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=C6906327&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6906327&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>affp:</b>    | Proton affinity                                 |
| <b>basg:</b>    | Gas basicity                                    |
| <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>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                   |
| <b>vc:</b>      | Critical Volume                                 |

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