

# (E)-3-(Dimethylamino)-2-pentene

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | (E)-C <sub>2</sub> H <sub>5</sub> C(N(CH <sub>3</sub> ) <sub>2</sub> )=CHCH <sub>3</sub>                 |
| <b>Inchi:</b>               | InChI=1S/C <sub>7</sub> H <sub>15</sub> N/c1-5-7(6-2)8(3)4/h5H,6H <sub>2</sub> ,1-4H <sub>3</sub> /b7-5- |
| <b>InchiKey:</b>            | UCCDUMHVMOCMTB-ALCCZGGFSA-N  |
| <b>Formula:</b>             | C <sub>7</sub> H <sub>15</sub> N   |
| <b>SMILES:</b>              | CC=C(CC)N(C)C  |
| <b>Mol. weight [g/mol]:</b> | 113.20   |
| <b>CAS:</b>                 | 32317-47-8   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 190.51  | kJ/mol               | Joback Method  |
| hf            | -12.85  | kJ/mol               | Joback Method  |
| hfus          | 15.80   | kJ/mol               | Joback Method  |
| hvap          | 33.26   | kJ/mol               | Joback Method  |
| ie            | 7.61    | eV                   | NIST Webbook   |
| log10ws       | -1.67   |                      | Crippen Method |
| logp          | 1.862   |                      | Crippen Method |
| mcvol         | 115.170 | ml/mol               | McGowan Method |
| pc            | 2969.80 | kPa                  | Joback Method  |
| tb            | 376.04  | K                    | Joback Method  |
| tc            | 550.51  | K                    | Joback Method  |
| tf            | 182.08  | K                    | Joback Method  |
| vc            | 0.426   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 207.42 | J/mol×K | 376.04          | Joback Method |
| cpg           | 220.54 | J/mol×K | 405.12          | Joback Method |
| cpg           | 233.05 | J/mol×K | 434.20          | Joback Method |
| cpg           | 244.97 | J/mol×K | 463.28          | Joback Method |
| cpg           | 256.32 | J/mol×K | 492.36          | Joback Method |
| cpg           | 267.13 | J/mol×K | 521.44          | Joback Method |
| cpg           | 277.42 | J/mol×K | 550.51          | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C32317478&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C32317478&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>                                     |
| <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>                         |

# 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>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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