

# Hexanal, 3-methyl-

|                      |  |
|----------------------|--|
| Other names:         | 3-Methylhexanal                                    |
| Inchi:               | InChI=1S/C7H14O/c1-3-4-7(2)5-6-8/h6-7H,3-5H2,1-2H3 |
| InchiKey:            | ZSJUABCTGCNBPF-UHFFFAOYSA-N                        |
| Formula:             | C7H14O   |
| SMILES:              | CCCC(C)CC=O  |
| Mol. weight [g/mol]: | 114.19   |
| CAS:                 | 19269-28-4   |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -93.90  | kJ/mol  | Joback Method  |
| hf            | -278.67 | kJ/mol  | Joback Method  |
| hfus          | 12.65   | kJ/mol  | Joback Method  |
| hvap          | 37.51   | kJ/mol  | Joback Method  |
| log10ws       | -1.79   |         | Crippen Method |
| logp          | 2.012   |         | Crippen Method |
| mcvol         | 111.060 | ml/mol  | McGowan Method |
| pc            | 3059.17 | kPa     | Joback Method  |
| ripol         | 1116.00 |         | NIST Webbook   |
| tb            | 407.78  | K       | Joback Method  |
| tc            | 583.42  | K       | Joback Method  |
| tf            | 195.65  | K       | Joback Method  |
| vc            | 0.439   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 269.38 | J/molxK | 554.14          | Joback Method |
| cpg           | 216.97 | J/molxK | 407.78          | Joback Method |
| cpg           | 228.33 | J/molxK | 437.05          | Joback Method |
| cpg           | 239.24 | J/molxK | 466.33          | Joback Method |
| cpg           | 249.71 | J/molxK | 495.60          | Joback Method |
| cpg           | 259.76 | J/molxK | 524.87          | Joback Method |
| cpg           | 278.60 | J/molxK | 583.42          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpl   | 245.94    | J/molxK | 323.15 | NIST Webbook  |
| dvisc | 0.0003089 | Paxs    | 407.78 | Joback Method |
| dvisc | 0.0075086 | Paxs    | 195.65 | Joback Method |
| dvisc | 0.0029368 | Paxs    | 231.00 | Joback Method |
| dvisc | 0.0014738 | Paxs    | 266.36 | Joback Method |
| dvisc | 0.0008693 | Paxs    | 301.72 | Joback Method |
| dvisc | 0.0005728 | Paxs    | 337.07 | Joback Method |
| dvisc | 0.0004085 | Paxs    | 372.42 | Joback Method |
| hvapt | 42.80     | kJ/mol  | 365.50 | NIST Webbook  |

## Correlations

| Information                 | Value                         |
|-----------------------------|-------------------------------|
| Property code               | pvap                          |
| Equation                    | $\ln(P_{vp}) = A + B/(T + C)$ |
| Coeff. A                    | 1.54613e+01                   |
| Coeff. B                    | -3.90935e+03                  |
| Coeff. C                    | -5.63390e+01                  |
| Temperature range (K), min. | 313.98                        |
| Temperature range (K), max. | 441.51                        |

## 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=C19269284&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C19269284&amp;Units=SI</a>   |
| <b>The Yaws Handbook of Vapor Pressure:</b> | <a href="https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure">https://www.sciencedirect.com/book/9780128029992/the-yaws-handbook-of-vapor-pressure</a> |
| <b>Crippen Method:</b>                      | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>cpl:</b>   | Liquid phase heat capacity              |
| <b>dvisc:</b> | Dynamic viscosity                       |
| <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>hvapt:</b>   | Enthalpy of vaporization at a given temperature |
| <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>pvap:</b>    | Vapor pressure                                  |
| <b>ripol:</b>   | 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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