

# Pentane, 3-methoxy-

|                      |                                                |
|----------------------|------------------------------------------------|
| Other names:         | 1-Ethylpropyl methyl ether                     |
| Inchi:               | InChI=1S/C6H14O/c1-4-6(5-2)7-3/h6H,4-5H2,1-3H3 |
| InchiKey:            | CQRFEDVNTJTKFU-UHFFFAOYSA-N                    |
| Formula:             | C6H14O                                         |
| SMILES:              | CCC(CC)OC                                      |
| Mol. weight [g/mol]: | 102.17                                         |
| CAS:                 | 36839-67-5                                     |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -107.80 | kJ/mol  | Joback Method  |
| hf            | -304.67 | kJ/mol  | Joback Method  |
| hfus          | 8.96    | kJ/mol  | Joback Method  |
| hvap          | 30.97   | kJ/mol  | Joback Method  |
| log10ws       | -1.53   |         | Crippen Method |
| logp          | 1.821   |         | Crippen Method |
| mcvol         | 101.270 | ml/mol  | McGowan Method |
| pc            | 3076.16 | kPa     | Joback Method  |
| tb            | 358.66  | K       | Joback Method  |
| tc            | 527.06  | K       | Joback Method  |
| tf            | 164.61  | K       | Joback Method  |
| vc            | 0.384   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 181.69    | J/mol×K | 358.66          | Joback Method |
| cpg           | 192.17    | J/mol×K | 386.73          | Joback Method |
| cpg           | 202.35    | J/mol×K | 414.79          | Joback Method |
| cpg           | 212.24    | J/mol×K | 442.86          | Joback Method |
| cpg           | 221.82    | J/mol×K | 470.92          | Joback Method |
| cpg           | 231.12    | J/mol×K | 498.99          | Joback Method |
| cpg           | 240.11    | J/mol×K | 527.06          | Joback Method |
| dvisc         | 0.0064749 | Pa×s    | 164.61          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0023051 | Pa×s | 196.95 | Joback Method |
| dvisc | 0.0010982 | Pa×s | 229.29 | Joback Method |
| dvisc | 0.0006285 | Pa×s | 261.63 | Joback Method |
| dvisc | 0.0004067 | Pa×s | 293.98 | Joback Method |
| dvisc | 0.0002868 | Pa×s | 326.32 | Joback Method |
| dvisc | 0.0002155 | Pa×s | 358.66 | 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=C36839675&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C36839675&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>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas 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>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mccvol:</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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