

# CYCLOPENTENE, 3-METHOXY-

|                      |                                                    |
|----------------------|----------------------------------------------------|
| Inchi:               | InChI=1S/C6H10O/c1-7-6-4-2-3-5-6/h2,4,6H,3,5H2,1H3 |
| InchiKey:            | PUNAFIBTAHETMN-UHFFFAOYSA-N                        |
| Formula:             | C6H10O                                             |
| SMILES:              | COC1C=CCC1                                         |
| Mol. weight [g/mol]: | 98.14                                              |

## Physical Properties

| Property code | Value       | Unit    | Source             |
|---------------|-------------|---------|--------------------|
| af            | 0.2556      |         | Cheméo Relay (1.0) |
| hf            | -109.81     | kJ/mol  | Cheméo Relay (1.0) |
| hfus          | 7.64        | kJ/mol  | Joback Method      |
| hvap          | 37.58       | kJ/mol  | Cheméo Relay (1.0) |
| ie            | 9.45 ± 0.05 | eV      | NIST Webbook       |
| logp          | 1.351       |         | Crippen Method     |
| mcvol         | 86.110      | ml/mol  | McGowan Method     |
| pc            | 3930.78     | kPa     | Joback Method      |
| tb            | 376.74      | K       | Cheméo Relay (1.0) |
| tc            | 554.53      | K       | Cheméo Relay (1.0) |
| tf            | 157.36      | K       | Cheméo Relay (1.0) |
| vc            | 0.304       | m3/kmol | Cheméo Relay (1.0) |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 149.07    | J/mol×K | 373.54          | Joback Method |
| cpg           | 214.25    | J/mol×K | 570.82          | Joback Method |
| cpg           | 204.65    | J/mol×K | 537.94          | Joback Method |
| cpg           | 194.55    | J/mol×K | 505.06          | Joback Method |
| cpg           | 183.96    | J/mol×K | 472.18          | Joback Method |
| cpg           | 172.86    | J/mol×K | 439.30          | Joback Method |
| cpg           | 161.23    | J/mol×K | 406.42          | Joback Method |
| dvisc         | 0.0005045 | Pa×s    | 282.40          | Joback Method |
| dvisc         | 0.0002500 | Pa×s    | 373.54          | Joback Method |
| dvisc         | 0.0003031 | Pa×s    | 343.16          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003815 | Pa×s | 312.78 | Joback Method |
| dvisc | 0.0019874 | Pa×s | 191.27 | Joback Method |
| dvisc | 0.0007136 | Pa×s | 252.03 | Joback Method |
| dvisc | 0.0011102 | Pa×s | 221.65 | Joback Method |

## Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C39819744&Units=SI>

Joback Method:

[https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

McGowan Method:

<http://link.springer.com/article/10.1007/BF02311772>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

Crippen Method:

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## Legend

|               |                                                 |
|---------------|-------------------------------------------------|
| <b>af:</b>    | Acentric Factor                                 |
| <b>cpg:</b>   | Ideal gas heat capacity                         |
| <b>dvisc:</b> | Dynamic viscosity                               |
| <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>logp:</b>  | Octanol/Water partition coefficient             |
| <b>mccol:</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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