

# Cyclopentene,3-butyl-

|                      |                                                             |
|----------------------|-------------------------------------------------------------|
| Other names:         | 3-Butyl-1-cyclopentene<br>3-Butylcyclopentene-1             |
| Inchi:               | InChI=1S/C9H16/c1-2-3-6-9-7-4-5-8-9/h4,7,9H,2-3,5-6,8H2,1H3 |
| InchiKey:            | OCVYLEAVUIYGLL-UHFFFAOYSA-N                                 |
| Formula:             | C9H16                                                       |
| SMILES:              | CCCCC1C=CCC1                                                |
| Mol. weight [g/mol]: | 124.22                                                      |
| CAS:                 | 22531-00-6                                                  |

## Physical Properties

| Property code | Value       | Unit   | Source         |
|---------------|-------------|--------|----------------|
| gf            | 91.41       | kJ/mol | Joback Method  |
| hf            | -110.83     | kJ/mol | Joback Method  |
| hfus          | 14.22       | kJ/mol | Joback Method  |
| hvap          | 36.18       | kJ/mol | Joback Method  |
| ie            | 8.83 ± 0.02 | eV     | NIST Webbook   |
| log10ws       | -3.10       |        | Crippen Method |
| logp          | 3.143       |        | Crippen Method |
| mcvol         | 122.510     | ml/mol | McGowan Method |
| pc            | 2871.95     | kPa    | Joback Method  |
| rinpol        | 911.00      |        | NIST Webbook   |
| rinpol        | 910.00      |        | NIST Webbook   |
| rinpol        | 914.00      |        | NIST Webbook   |
| rinpol        | 914.30      |        | NIST Webbook   |
| rinpol        | 910.50      |        | NIST Webbook   |
| rinpol        | 910.00      |        | NIST Webbook   |
| rinpol        | 914.00      |        | NIST Webbook   |
| rinpol        | 911.00      |        | NIST Webbook   |
| rinpol        | 916.00      |        | NIST Webbook   |
| rinpol        | 939.00      |        | NIST Webbook   |
| rinpol        | 944.00      |        | NIST Webbook   |
| ripol         | 1042.40     |        | NIST Webbook   |
| ripol         | 1042.00     |        | NIST Webbook   |
| ripol         | 1028.10     |        | NIST Webbook   |
| ripol         | 1036.60     |        | NIST Webbook   |
| ripol         | 1027.50     |        | NIST Webbook   |
| ripol         | 1028.10     |        | NIST Webbook   |

|       |               |         |               |
|-------|---------------|---------|---------------|
| ripol | 1036.60       |         | NIST Webbook  |
| ripol | 1042.60       |         | NIST Webbook  |
| ripol | 1039.10       |         | NIST Webbook  |
| ripol | 1035.70       |         | NIST Webbook  |
| ripol | 1042.40       |         | NIST Webbook  |
| ripol | 1031.60       |         | NIST Webbook  |
| ripol | 1028.00       |         | NIST Webbook  |
| ripol | 1023.00       |         | NIST Webbook  |
| ripol | 1043.00       |         | NIST Webbook  |
| ripol | 1039.00       |         | NIST Webbook  |
| ripol | 1036.00       |         | NIST Webbook  |
| ripol | 1032.00       |         | NIST Webbook  |
| ripol | 1035.00       |         | NIST Webbook  |
| ripol | 1046.00       |         | NIST Webbook  |
| ripol | 1042.00       |         | NIST Webbook  |
| ripol | 1049.00       |         | NIST Webbook  |
| ripol | 1022.90       |         | NIST Webbook  |
| ripol | 1027.00       |         | NIST Webbook  |
| tb    | 424.80 ± 0.70 | K       | NIST Webbook  |
| tc    | 612.82        | K       | Joback Method |
| tf    | 202.85        | K       | Joback Method |
| vc    | 0.467         | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 242.32    | J/mol×K | 419.76          | Joback Method |
| cpg           | 316.25    | J/mol×K | 580.64          | Joback Method |
| cpg           | 302.97    | J/mol×K | 548.47          | Joback Method |
| cpg           | 288.97    | J/mol×K | 516.29          | Joback Method |
| cpg           | 274.21    | J/mol×K | 484.11          | Joback Method |
| cpg           | 258.67    | J/mol×K | 451.94          | Joback Method |
| cpg           | 328.83    | J/mol×K | 612.82          | Joback Method |
| dvisc         | 0.0002955 | Pa×s    | 419.76          | Joback Method |
| dvisc         | 0.0003676 | Pa×s    | 383.61          | Joback Method |
| dvisc         | 0.0004787 | Pa×s    | 347.46          | Joback Method |
| dvisc         | 0.0006626 | Pa×s    | 311.31          | Joback Method |
| dvisc         | 0.0009991 | Pa×s    | 275.15          | Joback Method |
| dvisc         | 0.0017058 | Pa×s    | 239.00          | Joback Method |
| dvisc         | 0.0035241 | Pa×s    | 202.85          | Joback Method |

# Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C22531006&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C22531006&amp;Units=SI</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>                             |
| <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>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>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>rinpol:</b>  | Non-polar retention indices                     |
| <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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