

# Butane, 2-cyclopropyl-

|                      |                                                   |
|----------------------|---------------------------------------------------|
| Other names:         | Cyclopropane, sec-butyl-<br>sec-Butylcyclopropane |
| Inchi:               | InChI=1S/C7H14/c1-3-6(2)7-4-5-7/h6-7H,3-5H2,1-2H3 |
| InchiKey:            | INSSHDIMRIMVLZ-UHFFFAOYSA-N                       |
| Formula:             | C7H14                                             |
| SMILES:              | CCC(C)C1CC1                                       |
| Mol. weight [g/mol]: | 98.19                                             |
| CAS:                 | 5750-02-7                                         |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| chl           | -4372.00      | kJ/mol  | NIST Webbook   |
| gf            | 66.37         | kJ/mol  | Joback Method  |
| hf            | -120.29       | kJ/mol  | Joback Method  |
| hfus          | 8.50          | kJ/mol  | Joback Method  |
| hvap          | 30.70         | kJ/mol  | Joback Method  |
| log10ws       | -2.16         |         | Crippen Method |
| logp          | 2.442         |         | Crippen Method |
| mcvol         | 98.630        | ml/mol  | McGowan Method |
| pc            | 3257.86       | kPa     | Joback Method  |
| tb            | 364.13 ± 0.10 | K       | NIST Webbook   |
| tc            | 548.36        | K       | Joback Method  |
| tf            | 171.59        | K       | Joback Method  |
| vc            | 0.379         | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 177.35 | J/mol×K | 365.86          | Joback Method |
| cpg           | 191.27 | J/mol×K | 396.28          | Joback Method |
| cpg           | 204.50 | J/mol×K | 426.69          | Joback Method |
| cpg           | 217.06 | J/mol×K | 457.11          | Joback Method |
| cpg           | 228.97 | J/mol×K | 487.53          | Joback Method |
| cpg           | 240.28 | J/mol×K | 517.94          | Joback Method |

|       |           |         |        |               |
|-------|-----------|---------|--------|---------------|
| cpg   | 251.00    | J/mol×K | 548.36 | Joback Method |
| dvisc | 0.0014366 | Pa×s    | 171.59 | Joback Method |
| dvisc | 0.0009117 | Pa×s    | 203.97 | Joback Method |
| dvisc | 0.0006553 | Pa×s    | 236.35 | Joback Method |
| dvisc | 0.0005101 | Pa×s    | 268.73 | Joback Method |
| dvisc | 0.0004190 | Pa×s    | 301.10 | Joback Method |
| dvisc | 0.0003576 | Pa×s    | 333.48 | Joback Method |
| dvisc | 0.0003139 | Pa×s    | 365.86 | Joback Method |

## 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=C5750027&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5750027&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>                                   |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.com/doc/models/crippen_log10ws</a>                           |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>chl:</b>     | Standard liquid enthalpy of combustion          |
| <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>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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