

Cyclopentane, 1-butyl-1-methyl

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|----------------------|---|
| Inchi: | InChI=1S/C10H20/c1-3-4-7-10(2)8-5-6-9-10/h3-9H2,1-2H3 |
| InchiKey: | DMESIPKWNCPPMH-UHFFFAOYSA-N |
| Formula: | C10H20 |
| SMILES: | CCCCC1(C)CCCC1 |
| Mol. weight [g/mol]: | 140.27 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 64.38 | kJ/mol | Joback Method |
| hf | -174.01 | kJ/mol | Joback Method |
| hfus | 9.29 | kJ/mol | Joback Method |
| hvap | 36.96 | kJ/mol | Joback Method |
| log10ws | -3.66 | | Crippen Method |
| logp | 3.757 | | Crippen Method |
| mcvol | 140.900 | ml/mol | McGowan Method |
| pc | 2621.78 | kPa | Joback Method |
| rinpol | 991.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| rinpol | 987.00 | | NIST Webbook |
| rinpol | 991.00 | | NIST Webbook |
| rinpol | 982.00 | | NIST Webbook |
| tb | 443.72 | K | Joback Method |
| tc | 641.29 | K | Joback Method |
| tf | 237.26 | K | Joback Method |
| vc | 0.534 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 301.06 | J/molxK | 443.72 | Joback Method |
| cpg | 319.97 | J/molxK | 476.65 | Joback Method |
| cpg | 337.70 | J/molxK | 509.58 | Joback Method |
| cpg | 354.34 | J/molxK | 542.51 | Joback Method |

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|-----|--------|---------|--------|---------------|
| cpg | 370.00 | J/mol×K | 575.44 | Joback Method |
| cpg | 384.77 | J/mol×K | 608.36 | Joback Method |
| cpg | 398.74 | J/mol×K | 641.29 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=R10589&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

Latest version available from:

<https://www.chemeo.com/cid/67-450-8/Cyclopentane-1-butyl-1-methyl.pdf>

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