

trans-1-Butyl-2-methylcyclopropane

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| Other names: | 1-Butyl-2-methylcyclopropane, (E)- |
| Inchi: | InChI=1S/C8H16/c1-3-4-5-8-6-7(8)2/h7-8H,3-6H2,1-2H3/t7-,8-/m0/s1 |
| InchiKey: | IWTBNPKBPXCCIV-YUMQZZPRSA-N |
| Formula: | C8H16 |
| SMILES: | CCCCC1CC1C |
| Mol. weight [g/mol]: | 112.21 |
| CAS: | 38851-70-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 69.52 | kJ/mol | Joback Method |
| hf | -155.99 | kJ/mol | Joback Method |
| hfus | 15.68 | kJ/mol | Joback Method |
| hvap | 33.01 | kJ/mol | Joback Method |
| log10ws | -2.58 | | Crippen Method |
| logp | 2.833 | | Crippen Method |
| mcvol | 112.720 | ml/mol | McGowan Method |
| pc | 2802.44 | kPa | Joback Method |
| rinpol | 790.00 | | NIST Webbook |
| tb | 384.51 | K | Joback Method |
| tc | 561.42 | K | Joback Method |
| tf | 193.62 | K | Joback Method |
| vc | 0.440 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 216.48 | J/molxK | 384.51 | Joback Method |
| cpg | 284.10 | J/molxK | 531.93 | Joback Method |
| cpg | 271.82 | J/molxK | 502.45 | Joback Method |
| cpg | 258.93 | J/molxK | 472.96 | Joback Method |
| cpg | 245.43 | J/molxK | 443.48 | Joback Method |
| cpg | 231.29 | J/molxK | 413.99 | Joback Method |
| cpg | 295.82 | J/molxK | 561.42 | Joback Method |

| | | | | |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003249 | Paxs | 384.51 | Joback Method |
| dvisc | 0.0003486 | Paxs | 352.69 | Joback Method |
| dvisc | 0.0003793 | Paxs | 320.88 | Joback Method |
| dvisc | 0.0004205 | Paxs | 289.06 | Joback Method |
| dvisc | 0.0004781 | Paxs | 257.25 | Joback Method |
| dvisc | 0.0005637 | Paxs | 225.44 | Joback Method |
| dvisc | 0.0007016 | Paxs | 193.62 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C38851706&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| 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 |

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<https://www.chemeo.com/cid/61-375-8/trans-1-Butyl-2-methylcyclopropane.pdf>

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