

trans-3-t-Butylcyclobutanol

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|----------------------|---|
| Inchi: | InChI=1S/C8H16O/c1-8(2,3)6-4-7(9)5-6/h6-7,9H,4-5H2,1-3H3/t6-,7- |
| InchiKey: | QTUJAHPEPCHIKC-LJGSYFOKSA-N |
| Formula: | C8H16O |
| SMILES: | CC(C)(C)C1CC(O)C1 |
| Mol. weight [g/mol]: | 128.21 |
| CAS: | 20476-25-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -76.56 | kJ/mol | Joback Method |
| hf | -323.13 | kJ/mol | Joback Method |
| hfus | 10.26 | kJ/mol | Joback Method |
| hvap | 48.56 | kJ/mol | Joback Method |
| log10ws | -1.96 | | Crippen Method |
| logp | 1.803 | | Crippen Method |
| mcvol | 118.590 | ml/mol | McGowan Method |
| pc | 3254.14 | kPa | Joback Method |
| tb | 477.73 | K | Joback Method |
| tc | 665.75 | K | Joback Method |
| tf | 253.34 | K | Joback Method |
| vc | 0.440 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 278.61 | J/molxK | 477.73 | Joback Method |
| cpg | 293.25 | J/molxK | 509.07 | Joback Method |
| cpg | 307.08 | J/molxK | 540.40 | Joback Method |
| cpg | 320.13 | J/molxK | 571.74 | Joback Method |
| cpg | 332.43 | J/molxK | 603.08 | Joback Method |
| cpg | 344.04 | J/molxK | 634.41 | Joback Method |
| cpg | 354.98 | J/molxK | 665.75 | Joback Method |
| dvisc | 0.0277371 | Paxs | 253.34 | Joback Method |
| dvisc | 0.0078992 | Paxs | 290.74 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0029953 | Paxs | 328.14 | Joback Method |
| dvisc | 0.0013851 | Paxs | 365.53 | Joback Method |
| dvisc | 0.0007391 | Paxs | 402.93 | Joback Method |
| dvisc | 0.0004388 | Paxs | 440.33 | Joback Method |
| dvisc | 0.0002827 | Paxs | 477.73 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C20476259&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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 |
| mccvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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