

1,2-Cyclobutanedicarboxylic acid, trans-

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| Other names: | trans-1,2-Cyclobutanedicarboxylic Acid USAF st-3 1,2-Cyclobutanedicarboxylic acid, (E)- (E)-1,2-Cyclobutanedicarboxylic acid trans-cyclobutane-1,2-dicarboxylic acid |
| Inchi: | InChI=1S/C6H8O4/c7-5(8)3-1-2-4(3)6(9)10/h3-4H,1-2H2,(H,7,8)(H,9,10)/t3-,4-/m0/s1 |
| InchiKey: | SUSAGCZZQKACKE-IMJSIDKUSA-N |
| Formula: | C6H8O4 |
| SMILES: | O=C(O)C1CCC1C(=O)O |
| Mol. weight [g/mol]: | 144.13 |
| CAS: | 1124-13-6 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -490.90 | kJ/mol | Joback Method |
| hf | -650.49 | kJ/mol | Joback Method |
| hfus | 19.78 | kJ/mol | Joback Method |
| hvap | 75.58 | kJ/mol | Joback Method |
| log10ws | 0.06 | | Crippen Method |
| logp | 0.182 | | Crippen Method |
| mcvol | 99.420 | ml/mol | McGowan Method |
| pc | 5390.71 | kPa | Joback Method |
| tb | 635.12 | K | Joback Method |
| tc | 823.70 | K | Joback Method |
| tf | 389.06 | K | Joback Method |
| vc | 0.369 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 265.38 | J/molxK | 635.12 | Joback Method |
| cpg | 273.33 | J/molxK | 666.55 | Joback Method |
| cpg | 280.81 | J/molxK | 697.98 | Joback Method |
| cpg | 287.84 | J/molxK | 729.41 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 294.43 | J/molxK | 760.84 | Joback Method |
| cpg | 300.61 | J/molxK | 792.27 | Joback Method |
| cpg | 306.40 | J/molxK | 823.70 | Joback Method |
| dvisc | 0.0055272 | Paxs | 389.06 | Joback Method |
| dvisc | 0.0019472 | Paxs | 430.07 | Joback Method |
| dvisc | 0.0008226 | Paxs | 471.08 | Joback Method |
| dvisc | 0.0003989 | Paxs | 512.09 | Joback Method |
| dvisc | 0.0002154 | Paxs | 553.10 | Joback Method |
| dvisc | 0.0001266 | Paxs | 594.11 | Joback Method |
| dvisc | 0.0000797 | Paxs | 635.12 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C1124136&Units=SI |
| 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 |

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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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