

Cyclohexanol, 5-methyl-2-(1-methylethyl)-, (1 «alpha»,2 «alpha»,5 «alpha»)-

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|----------------------|---|
| Other names: | Menthol, cis-1,3,cis-1,4- Neoisomenthol Isoneomenthol 2-Isopropyl-5-methylcyclohexanol, (1 «alpha»,2 «alpha»,5 «alpha»)- |
| Inchi: | InChI=1S/C10H20O/c1-7(2)9-5-4-8(3)6-10(9)11/h7-11H,4-6H2,1-3H3/t8-,9-,10-/m0/s1 |
| InchiKey: | NOOLISFMXDJSKH-GUBZILKMSA-N |
| Formula: | C10H20O |
| SMILES: | CC1CCC(C(C)C)C(O)C1 |
| Mol. weight [g/mol]: | 156.27 |
| CAS: | 491-02-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|--------|----------------|
| gf | -96.91 | kJ/mol | Joback Method |
| hf | -393.60 | kJ/mol | Joback Method |
| hfus | 16.20 | kJ/mol | Joback Method |
| hvap | 53.96 | kJ/mol | Joback Method |
| log10ws | -2.55 | | Crippen Method |
| logp | 2.440 | | Crippen Method |
| mcvol | 146.770 | ml/mol | McGowan Method |
| pc | 2659.77 | kPa | Joback Method |
| rinpol | 1180.00 | | NIST Webbook |
| rinpol | 1193.00 | | NIST Webbook |
| rinpol | 1176.00 | | NIST Webbook |
| rinpol | 1194.00 | | NIST Webbook |
| rinpol | 1188.00 | | NIST Webbook |
| rinpol | 1183.00 | | NIST Webbook |
| rinpol | 1188.00 | | NIST Webbook |
| rinpol | 1188.00 | | NIST Webbook |
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| rinpol | 1182.00 | | NIST Webbook |
| rinpol | 1183.00 | | NIST Webbook |
| rinpol | 1186.00 | | NIST Webbook |
| rinpol | 1188.00 | | NIST Webbook |
| rinpol | 1192.00 | | NIST Webbook |
| rinpol | 1187.00 | | NIST Webbook |
| rinpol | 1189.00 | | NIST Webbook |

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| ripol | 1173.00 | | NIST Webbook |
| ripol | 1193.00 | | NIST Webbook |
| ripol | 1180.00 | | NIST Webbook |
| ripol | 1605.00 | | NIST Webbook |
| ripol | 1641.00 | | NIST Webbook |
| ripol | 1622.00 | | NIST Webbook |
| ripol | 1646.00 | | NIST Webbook |
| ripol | 1641.00 | | NIST Webbook |
| ripol | 1622.00 | | NIST Webbook |
| tb | 530.15 | K | Joback Method |
| tc | 719.67 | K | Joback Method |
| tf | 247.18 | K | Joback Method |
| vc | 0.539 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 370.36 | J/molxK | 530.15 | Joback Method |
| cpg | 387.84 | J/molxK | 561.74 | Joback Method |
| cpg | 404.52 | J/molxK | 593.32 | Joback Method |
| cpg | 420.40 | J/molxK | 624.91 | Joback Method |
| cpg | 435.50 | J/molxK | 656.49 | Joback Method |
| cpg | 449.82 | J/molxK | 688.08 | Joback Method |
| cpg | 463.40 | J/molxK | 719.67 | Joback Method |
| dvisc | 0.0430815 | Paxs | 247.18 | Joback Method |
| dvisc | 0.0077902 | Paxs | 294.34 | Joback Method |
| dvisc | 0.0022592 | Paxs | 341.50 | Joback Method |
| dvisc | 0.0008847 | Paxs | 388.66 | Joback Method |
| dvisc | 0.0004244 | Paxs | 435.83 | Joback Method |
| dvisc | 0.0002350 | Paxs | 482.99 | Joback Method |
| dvisc | 0.0001446 | Paxs | 530.15 | 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>

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 |
| rinpola: | Non-polar retention indices |
| ripola: | Polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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