

Benzenepentanol

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| Other names: | 1-pentanol, 5-phenyl- 5-Phenylpentanol 5-phenyl-1-pentanol 5-phenylpentan-1-ol Pentanol, 5-phenyl- Phenylamyl alcohol Phenylpentanol |
| Inchi: | InChI=1S/C11H16O/c12-10-6-2-5-9-11-7-3-1-4-8-11/h1,3-4,7-8,12H,2,5-6,9-10H2 |
| InchiKey: | DPZMVZIQRMVBBW-UHFFFAOYSA-N |
| Formula: | C11H16O |
| SMILES: | OCCCCC1CCCC1 |
| Mol. weight [g/mol]: | 164.24 |
| CAS: | 10521-91-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 17.33 | kJ/mol | Joback Method |
| hf | -186.07 | kJ/mol | Joback Method |
| hfus | 22.38 | kJ/mol | Joback Method |
| hvap | 59.03 | kJ/mol | Joback Method |
| log10ws | -2.79 | | Crippen Method |
| logp | 2.392 | | Crippen Method |
| mcvol | 147.960 | ml/mol | McGowan Method |
| pc | 2918.68 | kPa | Joback Method |
| tb | 569.94 | K | Joback Method |
| tc | 759.99 | K | Joback Method |
| tf | 300.97 | K | Joback Method |
| vc | 0.562 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 358.48 | J/mol×K | 569.94 | Joback Method |
| cpg | 371.72 | J/mol×K | 601.61 | Joback Method |

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|-------|-----------|---------|--------|---------------|
| cpg | 384.25 | J/molxK | 633.29 | Joback Method |
| cpg | 396.09 | J/molxK | 664.96 | Joback Method |
| cpg | 407.28 | J/molxK | 696.64 | Joback Method |
| cpg | 417.84 | J/molxK | 728.31 | Joback Method |
| cpg | 427.81 | J/molxK | 759.99 | Joback Method |
| dvisc | 0.0116411 | Paxs | 300.97 | Joback Method |
| dvisc | 0.0030637 | Paxs | 345.80 | Joback Method |
| dvisc | 0.0010954 | Paxs | 390.63 | Joback Method |
| dvisc | 0.0004840 | Paxs | 435.45 | Joback Method |
| dvisc | 0.0002491 | Paxs | 480.28 | Joback Method |
| dvisc | 0.0001436 | Paxs | 525.11 | Joback Method |
| dvisc | 0.0000903 | Paxs | 569.94 | Joback Method |
| hvapt | 58.20 | kJ/mol | 401.50 | NIST Webbook |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|--------|------|----------------|--------------|
| tbrp | 428.20 | K | 2.70 | NIST Webbook |

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=C10521912&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Partitioning of Phenylalkanols between Micelles and Water Studied by Limiting Interdiffusion Coefficients in Water and Tetradecyltrimethylammonium Bromide Solutions: <https://www.doi.org/10.1021/je900967j>

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 |

| | |
|---------------------------------------|-------------------------------------------------|
| h_{vap}: | Enthalpy of vaporization at standard conditions |
| h_{vapt}: | Enthalpy of vaporization at a given temperature |
| log₁₀w_s: | Log10 of Water solubility in mol/l |
| log_p: | Octanol/Water partition coefficient |
| mc_{vol}: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| tb: | Normal Boiling Point Temperature |
| t_{brp}: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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