

1-Propanol, dl-2-benzylamino-

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| Inchi: | InChI=1S/C10H15NO/c1-9(8-12)11-7-10-5-3-2-4-6-10/h2-6,9,11-12H,7-8H2,1H3 |
| InchiKey: | PJXWCRXOPLGFLX-UHFFFAOYSA-N |
| Formula: | C10H15NO |
| SMILES: | CC(CO)NCc1ccccc1 |
| Mol. weight [g/mol]: | 165.23 |
| CAS: | 6940-81-4 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 95.86 | kJ/mol | Joback Method |
| hf | -117.24 | kJ/mol | Joback Method |
| hfus | 21.36 | kJ/mol | Joback Method |
| hvap | 62.86 | kJ/mol | Joback Method |
| log10ws | -2.17 | | Crippen Method |
| logp | 1.157 | | Crippen Method |
| mcvol | 143.850 | ml/mol | McGowan Method |
| pc | 3325.84 | kPa | Joback Method |
| tb | 596.79 | K | Joback Method |
| tc | 794.00 | K | Joback Method |
| tf | 327.36 | K | Joback Method |
| vc | 0.535 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 360.60 | J/mol×K | 596.79 | Joback Method |
| cpg | 373.31 | J/mol×K | 629.66 | Joback Method |
| cpg | 385.28 | J/mol×K | 662.53 | Joback Method |
| cpg | 396.53 | J/mol×K | 695.39 | Joback Method |
| cpg | 407.11 | J/mol×K | 728.26 | Joback Method |
| cpg | 417.04 | J/mol×K | 761.13 | Joback Method |
| cpg | 426.35 | J/mol×K | 794.00 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C6940814&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| 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 |
| 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 |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| m cvol: | 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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