

2,5-Diethoxyaniline

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| Other names: | Aminohydroquinone diethyl ether Benzenamine, 2,5-diethoxy- Aniline, 2,5-diethoxy- |
| Inchi: | InChI=1S/C10H15NO2/c1-3-12-8-5-6-10(13-4-2)9(11)7-8/h5-7H,3-4,11H2,1-2H3 |
| InchiKey: | XPKFTIYOZUJAGA-UHFFFAOYSA-N |
| Formula: | C10H15NO2 |
| SMILES: | CCOc1ccc(OCC)c(N)c1 |
| Mol. weight [g/mol]: | 181.23 |
| CAS: | 94-85-9 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -17.08 | kJ/mol | Joback Method |
| hf | -266.79 | kJ/mol | Joback Method |
| hfus | 22.49 | kJ/mol | Joback Method |
| hvap | 56.92 | kJ/mol | Joback Method |
| log10ws | -2.18 | | Crippen Method |
| logp | 2.066 | | Crippen Method |
| mcvol | 149.720 | ml/mol | McGowan Method |
| pc | 2909.25 | kPa | Joback Method |
| tb | 582.21 | K | Joback Method |
| tc | 795.30 | K | Joback Method |
| tf | 381.64 | K | Joback Method |
| vc | 0.552 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 364.65 | J/molxK | 582.21 | Joback Method |
| cpg | 378.45 | J/molxK | 617.72 | Joback Method |
| cpg | 391.58 | J/molxK | 653.24 | Joback Method |
| cpg | 404.04 | J/molxK | 688.75 | Joback Method |
| cpg | 415.81 | J/molxK | 724.27 | Joback Method |
| cpg | 426.90 | J/molxK | 759.78 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C94859&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| 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 |
| 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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