

2-(N-Ethyl-N-toluidino)ethanol, methyl ether

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|-----------------------------|---|
| Inchi: | InChI=1S/C12H19NO/c1-4-13(8-9-14-3)12-7-5-6-11(2)10-12/h5-7,10H,4,8-9H2,1-3H3 |
| InchiKey: | QCQGUVVRXARGPG-UHFFFAOYSA-N |
| Formula: | C12H19NO |
| SMILES: | CCN(CCOC)c1cccc(C)c1 |
| Mol. weight [g/mol]: | 193.29 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 158.72 | kJ/mol | Joback Method |
| hf | -130.64 | kJ/mol | Joback Method |
| hfus | 24.70 | kJ/mol | Joback Method |
| hvap | 49.70 | kJ/mol | Joback Method |
| log10ws | -2.20 | | Crippen Method |
| logp | 2.468 | | Crippen Method |
| mcvol | 172.030 | ml/mol | McGowan Method |
| pc | 2327.03 | kPa | Joback Method |
| rinsol | 1508.10 | | NIST Webbook |
| tb | 540.48 | K | Joback Method |
| tc | 736.72 | K | Joback Method |
| tf | 318.64 | K | Joback Method |
| vc | 0.635 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 407.81 | J/mol×K | 540.48 | Joback Method |
| cpg | 424.51 | J/mol×K | 573.19 | Joback Method |
| cpg | 440.36 | J/mol×K | 605.89 | Joback Method |
| cpg | 455.38 | J/mol×K | 638.60 | Joback Method |
| cpg | 469.60 | J/mol×K | 671.31 | Joback Method |
| cpg | 483.05 | J/mol×K | 704.01 | Joback Method |
| cpg | 495.74 | J/mol×K | 736.72 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U333798&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 |
| 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 |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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