

N,N-Diethyl-3-nitroaniline

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| Other names: | N,N-Diethyl-m-nitroaniline Benzenamine, N,N-diethyl-3-nitro- |
| Inchi: | InChI=1S/C10H14N2O2/c1-3-11(4-2)9-6-5-7-10(8-9)12(13)14/h5-8H,3-4H2,1-2H3 |
| InchiKey: | QSNHMSRICSDACJ-UHFFFAOYSA-N |
| Formula: | C10H14N2O2 |
| SMILES: | CCN(CC)c1cccc([N+](=O)[O-])c1 |
| Mol. weight [g/mol]: | 194.23 |
| CAS: | 2216-16-2 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 282.43 | kJ/mol | Joback Method |
| hf | 32.10 | kJ/mol | Joback Method |
| hfus | 29.69 | kJ/mol | Joback Method |
| hvap | 59.43 | kJ/mol | Joback Method |
| log10ws | -2.87 | | Crippen Method |
| logp | 2.441 | | Crippen Method |
| mvol | 155.400 | ml/mol | McGowan Method |
| pc | 2915.53 | kPa | Joback Method |
| tb | 562.20 | K | NIST Webbook |
| tc | 854.90 | K | Joback Method |
| tf | 417.48 | K | Joback Method |
| vc | 0.588 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 394.46 | J/molxK | 624.14 | Joback Method |
| cpg | 408.90 | J/molxK | 662.60 | Joback Method |
| cpg | 422.31 | J/molxK | 701.06 | Joback Method |
| cpg | 434.76 | J/molxK | 739.52 | Joback Method |
| cpg | 446.29 | J/molxK | 777.98 | Joback Method |
| cpg | 456.97 | J/molxK | 816.44 | Joback Method |
| cpg | 466.85 | J/molxK | 854.90 | Joback Method |

Pressure Dependent Properties

| Property code | Value | Unit | Pressure [kPa] | Source |
|---------------|---------------|------|----------------|--------------|
| tbrp | 448.00 ± 1.00 | K | 2.40 | NIST Webbook |

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 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C2216162&Units=SI |

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 |
| tb: | Normal Boiling Point Temperature |
| tbrp: | Boiling point at reduced pressure |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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