

2-Nonenenitrile

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|-----------------------------|---|
| Other names: | non-2-enenitrile |
| Inchi: | InChI=1S/C9H15N/c1-2-3-4-5-6-7-8-9-10/h7-8H,2-6H2,1H3/b8-7+ |
| InchiKey: | WOVJAWMZNOWDII-BQYQJAHWSA-N |
| Formula: | C9H15N |
| SMILES: | CCCCCCC=CC#N |
| Mol. weight [g/mol]: | 137.22 |
| CAS: | 29127-83-1 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 238.30 | kJ/mol | Joback Method |
| hf | 53.01 | kJ/mol | Joback Method |
| hfus | 20.77 | kJ/mol | Joback Method |
| hvap | 46.06 | kJ/mol | Joback Method |
| log10ws | -3.31 | | Crippen Method |
| logp | 3.037 | | Crippen Method |
| mcvol | 134.750 | ml/mol | McGowan Method |
| pc | 2367.97 | kPa | Joback Method |
| rinpol | 1194.00 | | NIST Webbook |
| rinpol | 1194.00 | | NIST Webbook |
| tb | 511.56 | K | Joback Method |
| tc | 702.98 | K | Joback Method |
| tf | 251.10 | K | Joback Method |
| vc | 0.545 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 296.37 | J/molxK | 511.56 | Joback Method |
| cpg | 308.52 | J/molxK | 543.46 | Joback Method |
| cpg | 320.07 | J/molxK | 575.37 | Joback Method |
| cpg | 331.04 | J/molxK | 607.27 | Joback Method |
| cpg | 341.47 | J/molxK | 639.17 | Joback Method |
| cpg | 351.38 | J/molxK | 671.08 | Joback Method |

Sources

| | |
|------------------------|---|
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C29127831&Units=SI |
| 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 |

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 |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/28-504-1/2-Nonenenitrile.pdf>

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