

4,9-Dioxa-1,12-dodecanedinitrile

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|-----------------------------|---|
| Other names: | 3,3'-Tetramethylene-di-oxydipropionitrile 3,3'-[butane-1,4-diylbis(oxy)]bispropiononitrile |
| Inchi: | InChI=1S/C10H16N2O2/c11-5-3-9-13-7-1-2-8-14-10-4-6-12/h1-4,7-10H2 |
| InchiKey: | RCRNVWKZQROUJM-UHFFFAOYSA-N |
| Formula: | C10H16N2O2 |
| SMILES: | N#CCCOCCCCOCCC#N |
| Mol. weight [g/mol]: | 196.25 |
| CAS: | 18664-94-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | 89.68 | kJ/mol | Joback Method |
| hf | -184.41 | kJ/mol | Joback Method |
| hfus | 27.04 | kJ/mol | Joback Method |
| hvap | 63.63 | kJ/mol | Joback Method |
| log10ws | -1.92 | | Crippen Method |
| logp | 1.627 | | Crippen Method |
| mvol | 166.260 | ml/mol | McGowan Method |
| pc | 1954.41 | kPa | Joback Method |
| tb | 677.20 | K | Joback Method |
| tc | 871.10 | K | Joback Method |
| tf | 376.90 | K | Joback Method |
| vc | 0.683 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 438.01 | J/mol×K | 677.20 | Joback Method |
| cpg | 449.28 | J/mol×K | 709.52 | Joback Method |
| cpg | 459.99 | J/mol×K | 741.83 | Joback Method |
| cpg | 470.14 | J/mol×K | 774.15 | Joback Method |
| cpg | 479.73 | J/mol×K | 806.47 | Joback Method |
| cpg | 488.75 | J/mol×K | 838.79 | Joback Method |
| cpg | 497.21 | J/mol×K | 871.10 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=C18664943&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

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 |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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