

triethyl nitrilotricarboxylate

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| Inchi: | InChI=1S/C9H15NO6/c1-4-14-7(11)10(8(12)15-5-2)9(13)16-6-3/h4-6H2,1-3H3 |
| InchiKey: | WMXDFLUIDJYHMF-UHFFFAOYSA-N |
| Formula: | C9H15NO6 |
| SMILES: | CCOC(=O)N(C(=O)OCC)C(=O)OCC |
| Mol. weight [g/mol]: | 233.22 |
| CAS: | 3206-31-3 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | -566.08 | kJ/mol | Joback Method |
| hf | -895.96 | kJ/mol | Joback Method |
| hfus | 30.45 | kJ/mol | Joback Method |
| hvap | 65.14 | kJ/mol | Joback Method |
| log10ws | -1.68 | | Crippen Method |
| logp | 1.758 | | Crippen Method |
| mcvol | 169.970 | ml/mol | McGowan Method |
| pc | 2640.67 | kPa | Joback Method |
| tb | 646.63 | K | Joback Method |
| tc | 833.37 | K | Joback Method |
| tf | 440.14 | K | Joback Method |
| vc | 0.629 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 446.26 | J/molxK | 646.63 | Joback Method |
| cpg | 458.15 | J/molxK | 677.75 | Joback Method |
| cpg | 469.44 | J/molxK | 708.88 | Joback Method |
| cpg | 480.12 | J/molxK | 740.00 | Joback Method |
| cpg | 490.18 | J/molxK | 771.12 | Joback Method |
| cpg | 499.62 | J/molxK | 802.25 | Joback Method |
| cpg | 508.42 | J/molxK | 833.37 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=C3206313&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 |

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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