

# Nonanoic acid, 1,2-ethanediylbis(oxy-2,1-ethanediyl) ester

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | Triethyleneglycol dipelargonate<br>ethylenebis(oxyethylene) dinonanoate          |
| <b>Inchi:</b>               | InChI=1S/C24H46O6/c1-3-5-7-9-11-13-15-23(25)29-21-19-27-17-18-28-20-22-30-24(26) |
| <b>InchiKey:</b>            | UBQXQCCAPASFJR-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C24H46O6   |
| <b>SMILES:</b>              | CCCCCCCCC(=O)OCCOCCOCCOC(=O)CCCCCCCC   |
| <b>Mol. weight [g/mol]:</b> | 430.62   |
| <b>CAS:</b>                 | 106-06-9   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -526.64  | kJ/mol               | Joback Method  |
| hf            | -1292.73 | kJ/mol               | Joback Method  |
| hfus          | 65.87    | kJ/mol               | Joback Method  |
| hvap          | 92.15    | kJ/mol               | Joback Method  |
| log10ws       | -5.77    |                      | Crippen Method |
| logp          | 5.607    |                      | Crippen Method |
| mvol          | 375.640  | ml/mol               | McGowan Method |
| pc            | 833.38   | kPa                  | Joback Method  |
| tb            | 945.94   | K                    | Joback Method  |
| tc            | 1164.48  | K                    | Joback Method  |
| tf            | 549.02   | K                    | Joback Method  |
| vc            | 1.464    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 1281.28 | J/molxK | 945.94          | Joback Method |
| cpg           | 1300.77 | J/molxK | 982.36          | Joback Method |
| cpg           | 1318.43 | J/molxK | 1018.79         | Joback Method |
| cpg           | 1334.27 | J/molxK | 1055.21         | Joback Method |
| cpg           | 1348.29 | J/molxK | 1091.63         | Joback Method |
| cpg           | 1360.51 | J/molxK | 1128.05         | Joback Method |
| cpg           | 1370.94 | J/molxK | 1164.48         | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002410 | Paxs | 549.02 | Joback Method |
| dvisc | 0.0001202 | Paxs | 615.17 | Joback Method |
| dvisc | 0.0000686 | Paxs | 681.33 | Joback Method |
| dvisc | 0.0000433 | Paxs | 747.48 | Joback Method |
| dvisc | 0.0000294 | Paxs | 813.63 | Joback Method |
| dvisc | 0.0000212 | Paxs | 879.79 | Joback Method |
| dvisc | 0.0000160 | Paxs | 945.94 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C106069&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C106069&amp;Units=SI</a> |

## Legend

|                 |   |
|-----------------|---|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>   | Dynamic viscosity                               |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log10ws:</b> | Log10 of Water solubility in mol/l              |
| <b>logp:</b>    | Octanol/Water partition coefficient             |
| <b>mcvol:</b>   | McGowan's characteristic volume                 |
| <b>pc:</b>      | Critical Pressure                               |
| <b>tb:</b>      | Normal Boiling Point Temperature                |
| <b>tc:</b>      | Critical Temperature                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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