

# Diethylene glycol distearate

|                             |  |
|-----------------------------|--|
| <b>Other names:</b>         | oxydiethane-1,2-diyl distearate  |
| <b>Inchi:</b>               | InChI=1S/C40H78O5/c1-3-5-7-9-11-13-15-17-19-21-23-25-27-29-31-33-39(41)44-37-35- |
| <b>InchiKey:</b>            | YKDMBTQVKVEMSA-UHFFFAOYSA-N  |
| <b>Formula:</b>             | C40H78O5   |
| <b>SMILES:</b>              | CCCCCCCCCCCCCCCCCCCC(=O)OCCOCCOC(=O)CCCCCCCCCCCCCCCC                             |
| <b>Mol. weight [g/mol]:</b> | 639.04   |
| <b>CAS:</b>                 | 109-30-8   |

## Physical Properties

| Property code | Value    | Unit                 | Source         |
|---------------|----------|----------------------|----------------|
| gf            | -286.92  | kJ/mol               | Joback Method  |
| hf            | -1490.75 | kJ/mol               | Joback Method  |
| hfus          | 106.12   | kJ/mol               | Joback Method  |
| hvap          | 125.36   | kJ/mol               | Joback Method  |
| log10ws       | -13.38   |                      | Crippen Method |
| logp          | 12.612   |                      | Crippen Method |
| mcvol         | 595.210  | ml/mol               | McGowan Method |
| pc            | 402.73   | kPa                  | Joback Method  |
| tb            | 1289.60  | K                    | Joback Method  |
| tc            | 1862.10  | K                    | Joback Method  |
| tf            | 707.11   | K                    | Joback Method  |
| vc            | 2.341    | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 2288.69   | J/molxK | 1289.60         | Joback Method |
| cpg           | 2318.07   | J/molxK | 1385.02         | Joback Method |
| cpg           | 2336.37   | J/molxK | 1480.43         | Joback Method |
| cpg           | 2345.06   | J/molxK | 1575.85         | Joback Method |
| cpg           | 2345.60   | J/molxK | 1671.27         | Joback Method |
| cpg           | 2339.47   | J/molxK | 1766.69         | Joback Method |
| cpg           | 2328.15   | J/molxK | 1862.10         | Joback Method |
| dvisc         | 0.0000364 | Paxs    | 707.11          | Joback Method |

|       |           |      |         |               |
|-------|-----------|------|---------|---------------|
| dvisc | 0.0000157 | Paxs | 804.19  | Joback Method |
| dvisc | 0.0000081 | Paxs | 901.27  | Joback Method |
| dvisc | 0.0000047 | Paxs | 998.36  | Joback Method |
| dvisc | 0.0000031 | Paxs | 1095.44 | Joback Method |
| dvisc | 0.0000021 | Paxs | 1192.52 | Joback Method |
| dvisc | 0.0000016 | Paxs | 1289.60 | 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=C109308&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C109308&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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