

# Diethylmalonic acid, 2-methoxyethyl propyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C13H24O5/c1-5-8-17-11(14)13(6-2,7-3)12(15)18-10-9-16-4/h5-10H2,1-4H3 |
| InchiKey:            | KLHNIZCOZZBGOU-UHFFFAOYSA-N   |
| Formula:             | C13H24O5  |
| SMILES:              | CCCOC(=O)C(CC)(CC)C(=O)OCCOC  |
| Mol. weight [g/mol]: | 260.33  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -511.42 | kJ/mol  | Joback Method  |
| hf            | -942.22 | kJ/mol  | Joback Method  |
| hfus          | 28.77   | kJ/mol  | Joback Method  |
| hvap          | 63.96   | kJ/mol  | Joback Method  |
| log10ws       | -1.83   |         | Crippen Method |
| logp          | 1.936   |         | Crippen Method |
| mcvol         | 214.780 | ml/mol  | McGowan Method |
| pc            | 1777.34 | kPa     | Joback Method  |
| rinpol        | 1531.00 |         | NIST Webbook   |
| rinpol        | 1531.00 |         | NIST Webbook   |
| tb            | 668.61  | K       | Joback Method  |
| tc            | 852.22  | K       | Joback Method  |
| tf            | 405.24  | K       | Joback Method  |
| vc            | 0.819   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 599.16    | J/molxK | 668.61          | Joback Method |
| cpg           | 614.53    | J/molxK | 699.21          | Joback Method |
| cpg           | 629.11    | J/molxK | 729.81          | Joback Method |
| cpg           | 642.93    | J/molxK | 760.42          | Joback Method |
| cpg           | 655.98    | J/molxK | 791.02          | Joback Method |
| cpg           | 668.26    | J/molxK | 821.62          | Joback Method |
| cpg           | 679.79    | J/molxK | 852.22          | Joback Method |
| dvisc         | 0.0011570 | Paxs    | 405.24          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0006130 | Paxs | 449.13 | Joback Method |
| dvisc | 0.0003637 | Paxs | 493.03 | Joback Method |
| dvisc | 0.0002350 | Paxs | 536.92 | Joback Method |
| dvisc | 0.0001622 | Paxs | 580.82 | Joback Method |
| dvisc | 0.0001180 | Paxs | 624.72 | Joback Method |
| dvisc | 0.0000894 | Paxs | 668.61 | 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=U370670&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370670&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>rinpol:</b>  | Non-polar retention indices                     |
| <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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