

# Diethylmalonic acid, ethyl 3-ethylphenyl ester

Inchi:

InchiKey:

Formula:

SMILES:

Mol. weight [g/mol]:

InChI=1S/C17H24O4/c1-5-13-10-9-11-14(12-13)21-16(19)17(6-2,7-3)15(18)20-8-4/h9-12

SGPPDCHWYGDGOW-UHFFFAOYSA-N

C17H24O4

CCOC(=O)C(CC)(CC)C(=O)Oc1cccc(CC)c1

292.37

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -269.96 | kJ/mol  | Joback Method  |
| hf            | -667.50 | kJ/mol  | Joback Method  |
| hfus          | 31.60   | kJ/mol  | Joback Method  |
| hvap          | 73.39   | kJ/mol  | Joback Method  |
| log10ws       | -4.14   |         | Crippen Method |
| logp          | 3.524   |         | Crippen Method |
| mcvol         | 241.510 | ml/mol  | McGowan Method |
| pc            | 1703.31 | kPa     | Joback Method  |
| rinpol        | 1874.00 |         | NIST Webbook   |
| tb            | 769.37  | K       | Joback Method  |
| tc            | 977.67  | K       | Joback Method  |
| tf            | 467.03  | K       | Joback Method  |
| vc            | 0.916   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 706.20    | J/mol×K | 769.37          | Joback Method |
| cpg           | 721.92    | J/mol×K | 804.09          | Joback Method |
| cpg           | 736.56    | J/mol×K | 838.80          | Joback Method |
| cpg           | 750.15    | J/mol×K | 873.52          | Joback Method |
| cpg           | 762.72    | J/mol×K | 908.23          | Joback Method |
| cpg           | 774.31    | J/mol×K | 942.95          | Joback Method |
| cpg           | 784.95    | J/mol×K | 977.67          | Joback Method |
| dvisc         | 0.0007474 | Pa×s    | 467.03          | Joback Method |
| dvisc         | 0.0004108 | Pa×s    | 517.42          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0002511 | Pa×s | 567.81 | Joback Method |
| dvisc | 0.0001663 | Pa×s | 618.20 | Joback Method |
| dvisc | 0.0001172 | Pa×s | 668.59 | Joback Method |
| dvisc | 0.0000867 | Pa×s | 718.98 | Joback Method |
| dvisc | 0.0000668 | Pa×s | 769.37 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U370583&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U370583&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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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