

# Diethylmalonic acid, 4-chloro-3-methylphenyl hexyl ester

**Inchi:** InChI=1S/C20H29ClO4/c1-5-8-9-10-13-24-18(22)20(6-2,7-3)19(23)25-16-11-12-17(21)15  
**InchiKey:** LRLPJQKWDWBIMP-UHFFFAOYSA-N  
**Formula:** C20H29ClO4  
**SMILES:** CCCCCCOC(=O)C(CC)(CC)C(=O)Oc1ccc(Cl)c(C)c1  
**Mol. weight [g/mol]:** 368.89

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -266.26 | kJ/mol  | Joback Method  |
| hf            | -756.63 | kJ/mol  | Joback Method  |
| hfus          | 43.18   | kJ/mol  | Joback Method  |
| hvap          | 85.11   | kJ/mol  | Joback Method  |
| log10ws       | -6.17   |         | Crippen Method |
| logp          | 5.484   |         | Crippen Method |
| mcvol         | 296.020 | ml/mol  | McGowan Method |
| pc            | 1309.90 | kPa     | Joback Method  |
| rinpol        | 2335.00 |         | NIST Webbook   |
| tb            | 880.42  | K       | Joback Method  |
| tc            | 1091.11 | K       | Joback Method  |
| tf            | 543.28  | K       | Joback Method  |
| vc            | 1.133   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 904.87    | J/mol×K | 880.42          | Joback Method |
| cpg           | 919.87    | J/mol×K | 915.53          | Joback Method |
| cpg           | 933.72    | J/mol×K | 950.65          | Joback Method |
| cpg           | 946.46    | J/mol×K | 985.76          | Joback Method |
| cpg           | 958.13    | J/mol×K | 1020.88         | Joback Method |
| cpg           | 968.77    | J/mol×K | 1055.99         | Joback Method |
| cpg           | 978.42    | J/mol×K | 1091.11         | Joback Method |
| dvisc         | 0.0003763 | Pa×s    | 543.28          | Joback Method |
| dvisc         | 0.0002140 | Pa×s    | 599.47          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001340 | Pa×s | 655.66 | Joback Method |
| dvisc | 0.0000904 | Pa×s | 711.85 | Joback Method |
| dvisc | 0.0000646 | Pa×s | 768.04 | Joback Method |
| dvisc | 0.0000483 | Pa×s | 824.23 | Joback Method |
| dvisc | 0.0000375 | Pa×s | 880.42 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U369915&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U369915&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>                         |
| <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>                     |

## 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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