

# Glutaric acid, 2-(4-chlorophenyl)ethyl ethyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C15H19ClO4/c1-2-19-14(17)4-3-5-15(18)20-11-10-12-6-8-13(16)9-7-12/h6-9H |
| InchiKey:            | PBBOGSJDIIGIEW-UHFFFAOYSA-N  |
| Formula:             | C15H19ClO4   |
| SMILES:              | CCOC(=O)CCCC(=O)OCCc1ccc(Cl)cc1  |
| Mol. weight [g/mol]: | 298.76   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | -301.57 | kJ/mol               | Joback Method  |
| hf            | -633.21 | kJ/mol               | Joback Method  |
| hfus          | 38.03   | kJ/mol               | Joback Method  |
| hvap          | 74.62   | kJ/mol               | Joback Method  |
| log10ws       | -3.61   |                      | Crippen Method |
| logp          | 3.159   |                      | Crippen Method |
| mcvol         | 225.570 | ml/mol               | McGowan Method |
| pc            | 1911.91 | kPa                  | Joback Method  |
| rinpola       | 2220.00 |                      | NIST Webbook   |
| tb            | 764.27  | K                    | Joback Method  |
| tc            | 971.48  | K                    | Joback Method  |
| tf            | 471.99  | K                    | Joback Method  |
| vc            | 0.865   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 620.06    | J/molxK | 764.27          | Joback Method |
| cpg           | 633.75    | J/molxK | 798.81          | Joback Method |
| cpg           | 646.48    | J/molxK | 833.34          | Joback Method |
| cpg           | 658.28    | J/molxK | 867.88          | Joback Method |
| cpg           | 669.14    | J/molxK | 902.41          | Joback Method |
| cpg           | 679.09    | J/molxK | 936.95          | Joback Method |
| cpg           | 688.14    | J/molxK | 971.48          | Joback Method |
| dvisc         | 0.0007853 | Paxs    | 471.99          | Joback Method |
| dvisc         | 0.0004679 | Paxs    | 520.70          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0003046 | Paxs | 569.42 | Joback Method |
| dvisc | 0.0002121 | Paxs | 618.13 | Joback Method |
| dvisc | 0.0001558 | Paxs | 666.84 | Joback Method |
| dvisc | 0.0001193 | Paxs | 715.56 | Joback Method |
| dvisc | 0.0000945 | Paxs | 764.27 | Joback Method |

## Sources

|                        |   |
|------------------------|---|
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U377298&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U377298&amp;Units=SI</a> |
| <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>                     |

## 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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