

# Glutaric acid, di(2-ethylcyclohexyl) ester

Inchi:

lnchl=1S/C21H36O4/c1-3-16-10-5-7-12-18(16)24-20(22)14-9-15-21(23)25-19-13-8-6-11

InchiKey:

KEIQQKWAURBMFG-UHFFFAOYSA-N

Formula:

C21H36O4

SMILES:

CCC1CCCCC1OC(=O)CCCC(=O)OC1CCCCC1CC

Mol. weight [g/mol]:

352.51

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -308.42 | kJ/mol  | Joback Method  |
| hf            | -898.41 | kJ/mol  | Joback Method  |
| hfus          | 41.53   | kJ/mol  | Joback Method  |
| hvap          | 80.89   | kJ/mol  | Joback Method  |
| log10ws       | -5.87   |         | Crippen Method |
| logp          | 5.181   |         | Crippen Method |
| mcvol         | 299.910 | ml/mol  | McGowan Method |
| pc            | 1277.33 | kPa     | Joback Method  |
| rinpol        | 2419.00 |         | NIST Webbook   |
| tb            | 862.22  | K       | Joback Method  |
| tc            | 1075.00 | K       | Joback Method  |
| tf            | 477.03  | K       | Joback Method  |
| vc            | 1.123   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 1031.72   | J/mol×K | 862.22          | Joback Method |
| cpg           | 1116.31   | J/mol×K | 1039.53         | Joback Method |
| cpg           | 1102.90   | J/mol×K | 1004.07         | Joback Method |
| cpg           | 1087.75   | J/mol×K | 968.61          | Joback Method |
| cpg           | 1070.85   | J/mol×K | 933.15          | Joback Method |
| cpg           | 1052.18   | J/mol×K | 897.68          | Joback Method |
| cpg           | 1128.02   | J/mol×K | 1075.00         | Joback Method |
| dvisc         | 0.0000827 | Pa×s    | 862.22          | Joback Method |
| dvisc         | 0.0001071 | Pa×s    | 798.02          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0001453 | Pa×s | 733.82 | Joback Method |
| dvisc | 0.0002088 | Pa×s | 669.62 | Joback Method |
| dvisc | 0.0003242 | Pa×s | 605.43 | Joback Method |
| dvisc | 0.0005586 | Pa×s | 541.23 | Joback Method |
| dvisc | 0.0011145 | Pa×s | 477.03 | Joback Method |

## Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <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=U405481&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405481&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>                                 |

## 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                                 |

Latest version available from:

<https://www.chemeo.com/cid/80-325-2/Glutaric-acid-di-2-ethylcyclohexyl-ester.pdf>

Generated by Cheméo on 2025-12-19 06:51:33.644159095 +0000 UTC m=+5875291.174199749.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.