

# Glutaric acid, 2-norbornyl 2,2-dichloroethyl ester

|                      |   |
|----------------------|---|
| Inchi:               | InChI=1S/C14H20Cl2O4/c15-12(16)8-19-13(17)2-1-3-14(18)20-11-7-9-4-5-10(11)6-9/h9- |
| InchiKey:            | MSJQNNTYZJWUBW-UHFFFAOYSA-N   |
| Formula:             | C14H20Cl2O4   |
| SMILES:              | O=C(CCCC(=O)OC1CC2CCC1C2)OCC(Cl)Cl  |
| Mol. weight [g/mol]: | 323.21  |

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -325.45 | kJ/mol  | Joback Method  |
| hf            | -739.55 | kJ/mol  | Joback Method  |
| hfus          | 37.70   | kJ/mol  | Joback Method  |
| hvap          | 73.14   | kJ/mol  | Joback Method  |
| log10ws       | -3.74   |         | Crippen Method |
| logp          | 3.235   |         | Crippen Method |
| mcvol         | 225.760 | ml/mol  | McGowan Method |
| pc            | 1916.94 | kPa     | Joback Method  |
| rinpol        | 2161.00 |         | NIST Webbook   |
| rinpol        | 2161.00 |         | NIST Webbook   |
| tb            | 759.80  | K       | Joback Method  |
| tc            | 970.11  | K       | Joback Method  |
| tf            | 464.82  | K       | Joback Method  |
| vc            | 0.865   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value     | Unit    | Temperature [K] | Source        |
|---------------|-----------|---------|-----------------|---------------|
| cpg           | 656.25    | J/molxK | 759.80          | Joback Method |
| cpg           | 722.65    | J/molxK | 935.06          | Joback Method |
| cpg           | 711.24    | J/molxK | 900.01          | Joback Method |
| cpg           | 698.94    | J/molxK | 864.96          | Joback Method |
| cpg           | 685.70    | J/molxK | 829.90          | Joback Method |
| cpg           | 671.49    | J/molxK | 794.85          | Joback Method |
| cpg           | 733.24    | J/molxK | 970.11          | Joback Method |
| dvisc         | 0.0006356 | Paxs    | 759.80          | Joback Method |

|       |           |      |        |               |
|-------|-----------|------|--------|---------------|
| dvisc | 0.0007406 | Paxs | 710.64 | Joback Method |
| dvisc | 0.0008829 | Paxs | 661.47 | Joback Method |
| dvisc | 0.0010825 | Paxs | 612.31 | Joback Method |
| dvisc | 0.0013754 | Paxs | 563.15 | Joback Method |
| dvisc | 0.0018296 | Paxs | 513.98 | Joback Method |
| dvisc | 0.0025850 | Paxs | 464.82 | 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=U405489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U405489&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>                                 |

## Legend

|                            |   |
|----------------------------|---|
| <b>cp<sub>g</sub>:</b>     | Ideal gas heat capacity                         |
| <b>dvisc:</b>              | Dynamic viscosity                               |
| <b>g<sub>f</sub>:</b>      | Standard Gibbs free energy of formation         |
| <b>h<sub>f</sub>:</b>      | Enthalpy of formation at standard conditions    |
| <b>h<sub>fus</sub>:</b>    | Enthalpy of fusion at standard conditions       |
| <b>h<sub>vap</sub>:</b>    | Enthalpy of vaporization at standard conditions |
| <b>log<sub>10</sub>ws:</b> | Log <sub>10</sub> of Water solubility in mol/l  |
| <b>log<sub>p</sub>:</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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