

Glutaric acid, 3-chlorophenyl propyl ester

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|-----------------------------|---|
| Inchi: | InChI=1S/C14H17ClO4/c1-2-9-18-13(16)7-4-8-14(17)19-12-6-3-5-11(15)10-12/h3,5-6,10 |
| InchiKey: | XCUBOCQUUSFRLQ-UHFFFAOYSA-N |
| Formula: | C14H17ClO4 |
| SMILES: | CCCOC(=O)CCCC(=O)Oc1cccc(Cl)c1 |
| Mol. weight [g/mol]: | 284.74 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -309.99 | kJ/mol | Joback Method |
| hf | -612.57 | kJ/mol | Joback Method |
| hfus | 35.44 | kJ/mol | Joback Method |
| hvap | 72.39 | kJ/mol | Joback Method |
| log10ws | -3.84 | | Crippen Method |
| logp | 3.369 | | Crippen Method |
| mvol | 211.480 | ml/mol | McGowan Method |
| pc | 2083.12 | kPa | Joback Method |
| rinpol | 2089.00 | | NIST Webbook |
| tb | 741.39 | K | Joback Method |
| tc | 950.76 | K | Joback Method |
| tf | 460.72 | K | Joback Method |
| vc | 0.808 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 565.99 | J/molxK | 741.39 | Joback Method |
| cpg | 579.31 | J/molxK | 776.28 | Joback Method |
| cpg | 591.71 | J/molxK | 811.18 | Joback Method |
| cpg | 603.21 | J/molxK | 846.07 | Joback Method |
| cpg | 613.81 | J/molxK | 880.97 | Joback Method |
| cpg | 623.52 | J/molxK | 915.86 | Joback Method |
| cpg | 632.35 | J/molxK | 950.76 | Joback Method |
| dvisc | 0.0008524 | Paxs | 460.72 | Joback Method |
| dvisc | 0.0005150 | Paxs | 507.50 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0003387 | Paxs | 554.28 | Joback Method |
| dvisc | 0.0002378 | Paxs | 601.06 | Joback Method |
| dvisc | 0.0001757 | Paxs | 647.83 | Joback Method |
| dvisc | 0.0001353 | Paxs | 694.61 | Joback Method |
| dvisc | 0.0001076 | Paxs | 741.39 | Joback Method |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| Joback Method: | https://en.wikipedia.org/wiki/Joback_method |
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U358809&Units=SI |

Legend

| | |
|-----------------|---|
| cpg: | Ideal gas heat capacity |
| dvisc: | Dynamic viscosity |
| gf: | Standard Gibbs free energy of formation |
| hf: | Enthalpy of formation at standard conditions |
| hfus: | Enthalpy of fusion at standard conditions |
| hvap: | Enthalpy of vaporization at standard conditions |
| log10ws: | Log10 of Water solubility in mol/l |
| logp: | Octanol/Water partition coefficient |
| mcvol: | McGowan's characteristic volume |
| pc: | Critical Pressure |
| rinpol: | Non-polar retention indices |
| tb: | Normal Boiling Point Temperature |
| tc: | Critical Temperature |
| tf: | Normal melting (fusion) point |
| vc: | Critical Volume |

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<https://www.chemeo.com/cid/41-568-6/Glutaric-acid-3-chlorophenyl-propyl-ester.pdf>

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