

Glutaric acid, 3-chlorophenyl isopropyl ester

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

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -312.43 | kJ/mol | Joback Method |
| hf | -617.85 | kJ/mol | Joback Method |
| hfus | 31.92 | kJ/mol | Joback Method |
| hvap | 72.01 | kJ/mol | Joback Method |
| log10ws | -3.96 | | Crippen Method |
| logp | 3.367 | | Crippen Method |
| mvol | 211.480 | ml/mol | McGowan Method |
| pc | 2098.42 | kPa | Joback Method |
| rinpol | 1936.00 | | NIST Webbook |
| rinpol | 1936.00 | | NIST Webbook |
| tb | 740.95 | K | Joback Method |
| tc | 953.69 | K | Joback Method |
| tf | 445.72 | K | Joback Method |
| vc | 0.802 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 566.56 | J/molxK | 740.95 | Joback Method |
| cpg | 580.10 | J/molxK | 776.41 | Joback Method |
| cpg | 592.69 | J/molxK | 811.86 | Joback Method |
| cpg | 604.33 | J/molxK | 847.32 | Joback Method |
| cpg | 615.04 | J/molxK | 882.78 | Joback Method |
| cpg | 624.82 | J/molxK | 918.24 | Joback Method |
| cpg | 633.68 | J/molxK | 953.69 | Joback Method |
| dvisc | 0.0009754 | Paxs | 445.72 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0005515 | Paxs | 494.93 | Joback Method |
| dvisc | 0.0003457 | Paxs | 544.13 | Joback Method |
| dvisc | 0.0002341 | Paxs | 593.34 | Joback Method |
| dvisc | 0.0001683 | Paxs | 642.54 | Joback Method |
| dvisc | 0.0001268 | Paxs | 691.75 | Joback Method |
| dvisc | 0.0000992 | Paxs | 740.95 | Joback Method |

Sources

| | |
|------------------------|---|
| 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=U393379&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

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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