

Glutaric acid, di((2-chlorocyclohexyl)methyl) ester

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|----------------------|--|
| Inchi: | InChI=1S/C19H30Cl2O4/c20-16-8-3-1-6-14(16)12-24-18(22)10-5-11-19(23)25-13-15-7-2 |
| InchiKey: | GEHMIUGYRSJLQN-UHFFFAOYSA-N |
| Formula: | C19H30Cl2O4 |
| SMILES: | O=C(CCCC(=O)OCC1CCCCC1Cl)OCC1CCCCC1Cl |
| Mol. weight [g/mol]: | 393.35 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|----------------------|----------------|
| gf | -349.12 | kJ/mol | Joback Method |
| hf | -888.61 | kJ/mol | Joback Method |
| hfus | 44.75 | kJ/mol | Joback Method |
| hvap | 85.21 | kJ/mol | Joback Method |
| log10ws | -5.34 | | Crippen Method |
| logp | 4.838 | | Crippen Method |
| mcvol | 296.210 | ml/mol | McGowan Method |
| pc | 1392.29 | kPa | Joback Method |
| rinpola | 2952.00 | | NIST Webbook |
| rinpola | 2952.00 | | NIST Webbook |
| tb | 891.32 | K | Joback Method |
| tc | 1113.78 | K | Joback Method |
| tf | 514.33 | K | Joback Method |
| vc | 1.109 | m ³ /kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|-----------|---------|-----------------|---------------|
| cpg | 968.89 | J/molxK | 891.32 | Joback Method |
| cpg | 1037.76 | J/molxK | 1076.70 | Joback Method |
| cpg | 1027.49 | J/molxK | 1039.62 | Joback Method |
| cpg | 1015.49 | J/molxK | 1002.55 | Joback Method |
| cpg | 1001.74 | J/molxK | 965.47 | Joback Method |
| cpg | 986.21 | J/molxK | 928.40 | Joback Method |
| cpg | 1046.32 | J/molxK | 1113.78 | Joback Method |
| dvisc | 0.0000817 | Paxs | 891.32 | Joback Method |

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|-------|-----------|------|--------|---------------|
| dvisc | 0.0001048 | Paxs | 828.49 | Joback Method |
| dvisc | 0.0001401 | Paxs | 765.66 | Joback Method |
| dvisc | 0.0001973 | Paxs | 702.82 | Joback Method |
| dvisc | 0.0002972 | Paxs | 639.99 | Joback Method |
| dvisc | 0.0004893 | Paxs | 577.16 | Joback Method |
| dvisc | 0.0009101 | Paxs | 514.33 | Joback Method |

Sources

| | |
|------------------------|---|
| McGowan Method: | http://link.springer.com/article/10.1007/BF02311772 |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405453&Units=SI |
| 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 |

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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