# Glutaric acid, 1-cyclopentylethyl 8-chlorooctyl ester

**Inchi:** InChI=1S/C20H35ClO4/c1-17(18-11-6-7-12-18)25-20(23)14-10-13-19(22)24-16-9-5-3-2-4

**InchiKey:** CGQOEMDNIHAZIB-UHFFFAOYSA-N

**Formula:** C20H35ClO4

**SMILES:** CC(OC(=O)CCCC(=O)OCCCCCCCCCl)C1CCCC1

**Mol. weight [g/mol]:** 374.94

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -328.14 | kJ/mol | Joback Method |
| hf | -906.27 | kJ/mol | Joback Method |
| hfus | 47.74 | kJ/mol | Joback Method |
| hvap | 82.68 | kJ/mol | Joback Method |
| log10ws | -5.84 | | Crippen Method |
| logp | 5.401 | | Crippen Method |
| mcvol | 308.920 | ml/mol | McGowan Method |
| pc | 1193.17 | kPa | Joback Method |
| rinpol | 2667.00 | | NIST Webbook |
| rinpol | 2667.00 | | NIST Webbook |
| tb | 861.85 | K | Joback Method |
| tc | 1061.85 | K | Joback Method |
| tf | 485.30 | K | Joback Method |
| vc | 1.188 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 993.44 | J/mol×K | 861.85 | Joback Method |
| cpg | 1011.01 | J/mol×K | 895.18 | Joback Method |
| cpg | 1027.33 | J/mol×K | 928.52 | Joback Method |
| cpg | 1042.44 | J/mol×K | 961.85 | Joback Method |
| cpg | 1056.37 | J/mol×K | 995.18 | Joback Method |
| cpg | 1069.16 | J/mol×K | 1028.51 | Joback Method |
| cpg | 1080.82 | J/mol×K | 1061.85 | Joback Method |
| dvisc | 0.0009703 | Pa×s | 485.30 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004724 | Pa×s | 548.06 | Joback Method |
| dvisc | 0.0002667 | Pa×s | 610.82 | Joback Method |
| dvisc | 0.0001675 | Pa×s | 673.57 | Joback Method |
| dvisc | 0.0001138 | Pa×s | 736.33 | Joback Method |
| dvisc | 0.0000822 | Pa×s | 799.09 | Joback Method |
| dvisc | 0.0000623 | Pa×s | 861.85 | Joback Method |

# Sources

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|---|---|
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **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=U405469&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 |