# Glutaric acid, isohexyl 2,3,5,6-tetrachlorophenyl ester

**Inchi:** InChI=1S/C17H20Cl4O4/c1-10(2)5-4-8-24-13(22)6-3-7-14(23)25-17-15(20)11(18)9-12(19

**InchiKey:** NUJUXSBEAAGYLG-UHFFFAOYSA-N

**Formula:** C17H20Cl4O4

**SMILES:** CC(C)CCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl

**Mol. weight [g/mol]:** 430.15

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -351.85 | kJ/mol | Joback Method |
| hf | -761.40 | kJ/mol | Joback Method |
| hfus | 51.11 | kJ/mol | Joback Method |
| hvap | 93.82 | kJ/mol | Joback Method |
| log10ws | -6.91 | | Crippen Method |
| logp | 6.355 | | Crippen Method |
| mcvol | 290.470 | ml/mol | McGowan Method |
| pc | 1449.04 | kPa | Joback Method |
| rinpol | 2799.00 | | NIST Webbook |
| rinpol | 2799.00 | | NIST Webbook |
| tb | 936.82 | K | Joback Method |
| tc | 1159.26 | K | Joback Method |
| tf | 606.85 | K | Joback Method |
| vc | 1.117 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 797.00 | J/mol×K | 936.82 | Joback Method |
| cpg | 838.52 | J/mol×K | 1122.19 | Joback Method |
| cpg | 832.48 | J/mol×K | 1085.11 | Joback Method |
| cpg | 825.32 | J/mol×K | 1048.04 | Joback Method |
| cpg | 817.02 | J/mol×K | 1010.97 | Joback Method |
| cpg | 807.58 | J/mol×K | 973.89 | Joback Method |
| cpg | 843.45 | J/mol×K | 1159.26 | Joback Method |
| dvisc | 0.0000437 | Pa×s | 936.82 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000541 | Pa×s | 881.82 | Joback Method |
| dvisc | 0.0000688 | Pa×s | 826.83 | Joback Method |
| dvisc | 0.0000907 | Pa×s | 771.84 | Joback Method |
| dvisc | 0.0001247 | Pa×s | 716.84 | Joback Method |
| dvisc | 0.0001806 | Pa×s | 661.85 | Joback Method |
| dvisc | 0.0002799 | Pa×s | 606.85 | Joback Method |

# Sources

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|---|---|
| **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=U359320&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 |