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

**Inchi:** InChI=1S/C13H12Cl4O4/c1-2-20-9(18)4-3-5-10(19)21-13-11(16)7(14)6-8(15)12(13)17/h6

**InchiKey:** IAVQKSJQRTZTDI-UHFFFAOYSA-N

**Formula:** C13H12Cl4O4

**SMILES:** CCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)cc(Cl)c1Cl

**Mol. weight [g/mol]:** 374.04

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -383.09 | kJ/mol | Joback Method |
| hf | -673.56 | kJ/mol | Joback Method |
| hfus | 44.27 | kJ/mol | Joback Method |
| hvap | 85.31 | kJ/mol | Joback Method |
| log10ws | -5.48 | | Crippen Method |
| logp | 4.939 | | Crippen Method |
| mcvol | 234.110 | ml/mol | McGowan Method |
| pc | 1973.55 | kPa | Joback Method |
| rinpol | 2417.00 | | NIST Webbook |
| tb | 845.74 | K | Joback Method |
| tc | 1069.58 | K | Joback Method |
| tf | 576.77 | K | Joback Method |
| vc | 0.899 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 574.46 | J/mol×K | 845.74 | Joback Method |
| cpg | 583.87 | J/mol×K | 883.05 | Joback Method |
| cpg | 592.38 | J/mol×K | 920.35 | Joback Method |
| cpg | 599.96 | J/mol×K | 957.66 | Joback Method |
| cpg | 606.62 | J/mol×K | 994.96 | Joback Method |
| cpg | 612.34 | J/mol×K | 1032.27 | Joback Method |
| cpg | 617.13 | J/mol×K | 1069.58 | Joback Method |
| dvisc | 0.0003959 | Pa×s | 576.77 | Joback Method |
| dvisc | 0.0002795 | Pa×s | 621.60 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002067 | Pa×s | 666.43 | Joback Method |
| dvisc | 0.0001589 | Pa×s | 711.25 | Joback Method |
| dvisc | 0.0001260 | Pa×s | 756.08 | Joback Method |
| dvisc | 0.0001025 | Pa×s | 800.91 | Joback Method |
| dvisc | 0.0000852 | Pa×s | 845.74 | Joback Method |

# Sources

**NIST Webbook:** http://webbook.nist.gov/cgi/cbook.cgi?ID=U359315&Units=SI

**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

# 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