# Glutaric acid, hex-4-yn-3-yl 2,4,5-trichlorophenyl ester

**Inchi:** InChI=1S/C17H17Cl3O4/c1-3-6-11(4-2)23-16(21)7-5-8-17(22)24-15-10-13(19)12(18)9-14

**InchiKey:** XIIZFAUNSMFTFK-UHFFFAOYSA-N

**Formula:** C17H17Cl3O4

**SMILES:** CC#CC(CC)OC(=O)CCCC(=O)Oc1cc(Cl)c(Cl)cc1Cl

**Mol. weight [g/mol]:** 391.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -127.49 | kJ/mol | Joback Method |
| hf | -461.89 | kJ/mol | Joback Method |
| hfus | 50.42 | kJ/mol | Joback Method |
| hvap | 90.93 | kJ/mol | Joback Method |
| log10ws | -6.38 | | Crippen Method |
| logp | 5.068 | | Crippen Method |
| mcvol | 269.630 | ml/mol | McGowan Method |
| pc | 1714.61 | kPa | Joback Method |
| rinpol | 2603.00 | | NIST Webbook |
| rinpol | 2603.00 | | NIST Webbook |
| tb | 903.41 | K | Joback Method |
| tc | 1134.67 | K | Joback Method |
| tf | 670.51 | K | Joback Method |
| vc | 1.030 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 722.48 | J/mol×K | 903.41 | Joback Method |
| cpg | 733.53 | J/mol×K | 941.95 | Joback Method |
| cpg | 743.43 | J/mol×K | 980.50 | Joback Method |
| cpg | 752.17 | J/mol×K | 1019.04 | Joback Method |
| cpg | 759.78 | J/mol×K | 1057.59 | Joback Method |
| cpg | 766.25 | J/mol×K | 1096.13 | Joback Method |
| cpg | 771.60 | J/mol×K | 1134.67 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U392161&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 |
| **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 |