# Glutaric acid, 2,4,6-trichlorophenyl 3-methylbutyl ester

**Inchi:** InChI=1S/C16H19Cl3O4/c1-10(2)6-7-22-14(20)4-3-5-15(21)23-16-12(18)8-11(17)9-13(16

**InchiKey:** JNHTUTYGPWSTOV-UHFFFAOYSA-N

**Formula:** C16H19Cl3O4

**SMILES:** CC(C)CCOC(=O)CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

**Mol. weight [g/mol]:** 381.68

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -338.71 | kJ/mol | Joback Method |
| hf | -713.55 | kJ/mol | Joback Method |
| hfus | 44.71 | kJ/mol | Joback Method |
| hvap | 86.55 | kJ/mol | Joback Method |
| log10ws | -5.81 | | Crippen Method |
| logp | 5.312 | | Crippen Method |
| mcvol | 264.140 | ml/mol | McGowan Method |
| pc | 1627.22 | kPa | Joback Method |
| rinpol | 2456.00 | | NIST Webbook |
| rinpol | 2456.00 | | NIST Webbook |
| tb | 871.53 | K | Joback Method |
| tc | 1089.08 | K | Joback Method |
| tf | 553.14 | K | Joback Method |
| vc | 1.012 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 720.95 | J/mol×K | 871.53 | Joback Method |
| cpg | 768.76 | J/mol×K | 1052.82 | Joback Method |
| cpg | 761.28 | J/mol×K | 1016.56 | Joback Method |
| cpg | 752.77 | J/mol×K | 980.31 | Joback Method |
| cpg | 743.22 | J/mol×K | 944.05 | Joback Method |
| cpg | 732.62 | J/mol×K | 907.79 | Joback Method |
| cpg | 775.20 | J/mol×K | 1089.08 | Joback Method |
| dvisc | 0.0000584 | Pa×s | 871.53 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000729 | Pa×s | 818.46 | Joback Method |
| dvisc | 0.0000939 | Pa×s | 765.40 | Joback Method |
| dvisc | 0.0001255 | Pa×s | 712.34 | Joback Method |
| dvisc | 0.0001759 | Pa×s | 659.27 | Joback Method |
| dvisc | 0.0002614 | Pa×s | 606.20 | Joback Method |
| dvisc | 0.0004193 | Pa×s | 553.14 | Joback Method |

# Sources

| | |
|---|---|
| **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=U393309&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 |