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

**Inchi:** InChI=1S/C17H10Cl3F3O4/c18-8-6-9(19)17(10(20)7-8)27-14(25)3-1-2-13(24)26-12-5-4-1

**InchiKey:** BCTAKADCXXFIGJ-UHFFFAOYSA-N

**Formula:** C17H10Cl3F3O4

**SMILES:** O=C(CCCC(=O)Oc1c(Cl)cc(Cl)cc1Cl)Oc1ccc(F)c(F)c1F

**Mol. weight [g/mol]:** 441.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -828.76 | kJ/mol | Joback Method |
| hf | -1115.12 | kJ/mol | Joback Method |
| hfus | 52.94 | kJ/mol | Joback Method |
| hvap | 90.98 | kJ/mol | Joback Method |
| log10ws | -7.22 | | Crippen Method |
| logp | 5.745 | | Crippen Method |
| mcvol | 259.780 | ml/mol | McGowan Method |
| pc | 1690.72 | kPa | Joback Method |
| rinpol | 2679.00 | | NIST Webbook |
| rinpol | 2679.00 | | NIST Webbook |
| tb | 934.28 | K | Joback Method |
| tc | 1159.23 | K | Joback Method |
| tf | 645.16 | K | Joback Method |
| vc | 1.020 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 688.68 | J/mol×K | 934.28 | Joback Method |
| cpg | 696.77 | J/mol×K | 971.77 | Joback Method |
| cpg | 703.77 | J/mol×K | 1009.26 | Joback Method |
| cpg | 709.70 | J/mol×K | 1046.76 | Joback Method |
| cpg | 714.54 | J/mol×K | 1084.25 | Joback Method |
| cpg | 718.30 | J/mol×K | 1121.74 | Joback Method |
| cpg | 720.99 | J/mol×K | 1159.23 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393647&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 |