# Glutaric acid, cyclohexylmethyl 2,3,5-trichlorophenyl ester

**Inchi:** InChI=1S/C18H21Cl3O4/c19-13-9-14(20)18(21)15(10-13)25-17(23)8-4-7-16(22)24-11-12

**InchiKey:** FHUMFNYSRTWROK-UHFFFAOYSA-N

**Formula:** C18H21Cl3O4

**SMILES:** O=C(CCCC(=O)Oc1cc(Cl)cc(Cl)c1Cl)OCC1CCCCC1

**Mol. weight [g/mol]:** 407.72

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -294.98 | kJ/mol | Joback Method |
| hf | -695.23 | kJ/mol | Joback Method |
| hfus | 45.25 | kJ/mol | Joback Method |
| hvap | 91.82 | kJ/mol | Joback Method |
| log10ws | -6.54 | | Crippen Method |
| logp | 5.846 | | Crippen Method |
| mcvol | 281.460 | ml/mol | McGowan Method |
| pc | 1633.81 | kPa | Joback Method |
| rinpol | 2872.00 | | NIST Webbook |
| rinpol | 2872.00 | | NIST Webbook |
| tb | 937.28 | K | Joback Method |
| tc | 1171.74 | K | Joback Method |
| tf | 598.06 | K | Joback Method |
| vc | 1.063 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 826.52 | J/mol×K | 937.28 | Joback Method |
| cpg | 838.64 | J/mol×K | 976.36 | Joback Method |
| cpg | 849.27 | J/mol×K | 1015.43 | Joback Method |
| cpg | 858.44 | J/mol×K | 1054.51 | Joback Method |
| cpg | 866.18 | J/mol×K | 1093.58 | Joback Method |
| cpg | 872.51 | J/mol×K | 1132.66 | Joback Method |
| cpg | 877.44 | J/mol×K | 1171.74 | Joback Method |
| dvisc | 0.0003541 | Pa×s | 598.06 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002212 | Pa×s | 654.60 | Joback Method |
| dvisc | 0.0001489 | Pa×s | 711.13 | Joback Method |
| dvisc | 0.0001062 | Pa×s | 767.67 | Joback Method |
| dvisc | 0.0000794 | Pa×s | 824.21 | Joback Method |
| dvisc | 0.0000616 | Pa×s | 880.74 | Joback Method |
| dvisc | 0.0000493 | Pa×s | 937.28 | Joback Method |

# Sources

| | |
|---|---|
| **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=U392183&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |