# Glutaric acid, butyl pentachlorophenyl ester

**Inchi:** InChI=1S/C15H15Cl5O4/c1-2-3-7-23-8(21)5-4-6-9(22)24-15-13(19)11(17)10(16)12(18)14
**InchiKey:** ZBYQIWFGPZQMHF-UHFFFAOYSA-N
**Formula:** C15H15Cl5O4
**SMILES:** CCCCOC(=O)CCCC(=O)Oc1c(Cl)c(Cl)c(Cl)c(Cl)c1Cl
**Mol. weight [g/mol]:** 436.54

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -387.81 | kJ/mol | Joback Method |
| hf | -742.05 | kJ/mol | Joback Method |
| hfus | 53.26 | kJ/mol | Joback Method |
| hvap | 94.81 | kJ/mol | Joback Method |
| log10ws | -7.00 | | Crippen Method |
| logp | 6.373 | | Crippen Method |
| mcvol | 274.530 | ml/mol | McGowan Method |
| pc | 1606.42 | kPa | Joback Method |
| rinpol | 2794.00 | | NIST Webbook |
| rinpol | 2794.00 | | NIST Webbook |
| tb | 933.91 | K | Joback Method |
| tc | 1159.65 | K | Joback Method |
| tf | 641.75 | K | Joback Method |
| vc | 1.060 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 701.06 | J/mol×K | 933.91 | Joback Method |
| cpg | 709.88 | J/mol×K | 971.53 | Joback Method |
| cpg | 717.65 | J/mol×K | 1009.16 | Joback Method |
| cpg | 724.36 | J/mol×K | 1046.78 | Joback Method |
| cpg | 730.00 | J/mol×K | 1084.41 | Joback Method |
| cpg | 734.58 | J/mol×K | 1122.03 | Joback Method |
| cpg | 738.08 | J/mol×K | 1159.65 | Joback Method |
| dvisc | 0.0002519 | Pa×s | 641.75 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001793 | Pa×s | 690.44 | Joback Method |
| dvisc | 0.0001335 | Pa×s | 739.14 | Joback Method |
| dvisc | 0.0001031 | Pa×s | 787.83 | Joback Method |
| dvisc | 0.0000820 | Pa×s | 836.52 | Joback Method |
| dvisc | 0.0000669 | Pa×s | 885.22 | Joback Method |
| dvisc | 0.0000558 | Pa×s | 933.91 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U360254&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 |

# Legend

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|---|---|
| **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 |