# Glutaric acid, butyl pentafluorophenyl ester

**Inchi:** InChI=1S/C15H15F5O4/c1-2-3-7-23-8(21)5-4-6-9(22)24-15-13(19)11(17)10(16)12(18)14
**InchiKey:** VSONKIZBKGLMPV-UHFFFAOYSA-N
**Formula:** C15H15F5O4
**SMILES:** CCCCOC(=O)CCCC(=O)Oc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 354.27

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1302.21 | kJ/mol | Joback Method |
| hf | -1643.90 | kJ/mol | Joback Method |
| hfus | 47.68 | kJ/mol | Joback Method |
| hvap | 68.80 | kJ/mol | Joback Method |
| log10ws | -5.24 | | Crippen Method |
| logp | 3.801 | | Crippen Method |
| mcvol | 222.180 | ml/mol | McGowan Method |
| pc | 1556.12 | kPa | Joback Method |
| rinpol | 1806.00 | | NIST Webbook |
| rinpol | 1806.00 | | NIST Webbook |
| tb | 743.11 | K | Joback Method |
| tc | 922.01 | K | Joback Method |
| tf | 495.10 | K | Joback Method |
| vc | 0.905 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 628.88 | J/mol×K | 743.11 | Joback Method |
| cpg | 640.91 | J/mol×K | 772.93 | Joback Method |
| cpg | 652.27 | J/mol×K | 802.74 | Joback Method |
| cpg | 662.94 | J/mol×K | 832.56 | Joback Method |
| cpg | 672.92 | J/mol×K | 862.38 | Joback Method |
| cpg | 682.20 | J/mol×K | 892.19 | Joback Method |
| cpg | 690.77 | J/mol×K | 922.01 | 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=U359067&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 |
| **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 |