# Glutaric acid, hexyl 1-(pentafluorophenyl)ethyl ester

**Inchi:** InChI=1S/C19H23F5O4/c1-3-4-5-6-10-27-12(25)8-7-9-13(26)28-11(2)14-15(20)17(22)19

**InchiKey:** QYROSCFOAVAICX-UHFFFAOYSA-N

**Formula:** C19H23F5O4

**SMILES:** CCCCCCOC(=O)CCCC(=O)OC(C)c1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 410.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1270.97 | kJ/mol | Joback Method |
| hf | -1731.74 | kJ/mol | Joback Method |
| hfus | 54.51 | kJ/mol | Joback Method |
| hvap | 77.31 | kJ/mol | Joback Method |
| log10ws | -6.72 | | Crippen Method |
| logp | 5.280 | | Crippen Method |
| mcvol | 278.540 | ml/mol | McGowan Method |
| pc | 1180.09 | kPa | Joback Method |
| rinpol | 2124.00 | | NIST Webbook |
| rinpol | 2124.00 | | NIST Webbook |
| tb | 834.19 | K | Joback Method |
| tc | 1022.89 | K | Joback Method |
| tf | 525.18 | K | Joback Method |
| vc | 1.123 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 853.81 | J/mol×K | 834.19 | Joback Method |
| cpg | 867.81 | J/mol×K | 865.64 | Joback Method |
| cpg | 880.85 | J/mol×K | 897.09 | Joback Method |
| cpg | 892.92 | J/mol×K | 928.54 | Joback Method |
| cpg | 904.02 | J/mol×K | 959.99 | Joback Method |
| cpg | 914.16 | J/mol×K | 991.44 | Joback Method |
| cpg | 923.35 | J/mol×K | 1022.89 | Joback Method |

# Sources

| | |
|---|---|
| **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=U377000&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |