# Glutaric acid, 2-(pentafluorophenoxy)ethyl propyl ester

**Inchi:** InChI=1S/C16H17F5O5/c1-2-6-24-9(22)4-3-5-10(23)25-7-8-26-16-14(20)12(18)11(17)13

**InchiKey:** BNYKUABOBJSPJG-UHFFFAOYSA-N

**Formula:** C16H17F5O5

**SMILES:** CCCOC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F

**Mol. weight [g/mol]:** 384.30

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1398.79 | kJ/mol | Joback Method |
| hf | -1796.76 | kJ/mol | Joback Method |
| hfus | 51.45 | kJ/mol | Joback Method |
| hvap | 73.43 | kJ/mol | Joback Method |
| log10ws | -4.74 | | Crippen Method |
| logp | 3.428 | | Crippen Method |
| mcvol | 242.140 | ml/mol | McGowan Method |
| pc | 1426.15 | kPa | Joback Method |
| rinpol | 2062.00 | | NIST Webbook |
| tb | 788.41 | K | Joback Method |
| tc | 970.80 | K | Joback Method |
| tf | 528.60 | K | Joback Method |
| vc | 0.980 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 710.72 | J/mol×K | 788.41 | Joback Method |
| cpg | 723.13 | J/mol×K | 818.81 | Joback Method |
| cpg | 734.73 | J/mol×K | 849.21 | Joback Method |
| cpg | 745.52 | J/mol×K | 879.60 | Joback Method |
| cpg | 755.48 | J/mol×K | 910.00 | Joback Method |
| cpg | 764.58 | J/mol×K | 940.40 | Joback Method |
| cpg | 772.84 | J/mol×K | 970.80 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U377321&Units=SI |

# 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 |