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

**Inchi:** InChI=1S/C21H27F5O5/c1-2-3-4-5-6-7-11-29-14(27)9-8-10-15(28)30-12-13-31-21-19(25
**InchiKey:** ZLIUXOKGCXVXAG-UHFFFAOYSA-N
**Formula:** C21H27F5O5
**SMILES:** CCCCCCCCOC(=O)CCCC(=O)OCCOc1c(F)c(F)c(F)c(F)c1F
**Mol. weight [g/mol]:** 454.43

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1356.69 | kJ/mol | Joback Method |
| hf | -1899.96 | kJ/mol | Joback Method |
| hfus | 64.40 | kJ/mol | Joback Method |
| hvap | 84.56 | kJ/mol | Joback Method |
| log10ws | -6.83 | | Crippen Method |
| logp | 5.378 | | Crippen Method |
| mcvol | 312.590 | ml/mol | McGowan Method |
| pc | 1022.04 | kPa | Joback Method |
| rinpol | 2557.00 | | NIST Webbook |
| rinpol | 2557.00 | | NIST Webbook |
| tb | 902.81 | K | Joback Method |
| tc | 1106.22 | K | Joback Method |
| tf | 584.95 | K | Joback Method |
| vc | 1.260 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 999.57 | J/mol×K | 902.81 | Joback Method |
| cpg | 1014.16 | J/mol×K | 936.71 | Joback Method |
| cpg | 1027.44 | J/mol×K | 970.61 | Joback Method |
| cpg | 1039.42 | J/mol×K | 1004.51 | Joback Method |
| cpg | 1050.08 | J/mol×K | 1038.41 | Joback Method |
| cpg | 1059.43 | J/mol×K | 1072.31 | Joback Method |
| cpg | 1067.46 | J/mol×K | 1106.22 | Joback Method |

# Sources

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|---|---|
| **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=U377328&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |