# Glutaric acid, 2,2,3,3-tetrafluoropropyl 8-chlorooctyl ester

**Inchi:** InChI=1S/C16H25ClF4O4/c17-10-5-3-1-2-4-6-11-24-13(22)8-7-9-14(23)25-12-16(20,21)1

**InchiKey:** SPMOJZIGRAGHQA-UHFFFAOYSA-N

**Formula:** C16H25ClF4O4

**SMILES:** O=C(CCCC(=O)OCC(F)(F)C(F)F)OCCCCCCCCCl

**Mol. weight [g/mol]:** 392.81

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1174.77 | kJ/mol | Joback Method |
| hf | -1677.38 | kJ/mol | Joback Method |
| hfus | 48.35 | kJ/mol | Joback Method |
| hvap | 68.95 | kJ/mol | Joback Method |
| log10ws | -5.03 | | Crippen Method |
| logp | 4.723 | | Crippen Method |
| mcvol | 270.500 | ml/mol | McGowan Method |
| pc | 1229.42 | kPa | Joback Method |
| rinpol | 2137.00 | | NIST Webbook |
| rinpol | 2137.00 | | NIST Webbook |
| tb | 748.90 | K | Joback Method |
| tc | 922.10 | K | Joback Method |
| tf | 434.10 | K | Joback Method |
| vc | 1.083 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 797.91 | J/mol×K | 748.90 | Joback Method |
| cpg | 812.40 | J/mol×K | 777.77 | Joback Method |
| cpg | 826.08 | J/mol×K | 806.63 | Joback Method |
| cpg | 838.96 | J/mol×K | 835.50 | Joback Method |
| cpg | 851.08 | J/mol×K | 864.37 | Joback Method |
| cpg | 862.45 | J/mol×K | 893.23 | Joback Method |
| cpg | 873.09 | J/mol×K | 922.10 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U393456&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |