# Glutaric acid, 1,1,1-trifluoroprop-2-yl 2-methoxyphenyl ester

**Inchi:** InChI=1S/C15H17F3O5/c1-10(15(16,17)18)22-13(19)8-5-9-14(20)23-12-7-4-3-6-11(12)2

**InchiKey:** VXAKPNIVUWXVRQ-UHFFFAOYSA-N

**Formula:** C15H17F3O5

**SMILES:** COc1ccccc1OC(=O)CCCC(=O)OC(C)C(F)(F)F

**Mol. weight [g/mol]:** 334.29

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -978.67 | kJ/mol | Joback Method |
| hf | -1352.05 | kJ/mol | Joback Method |
| hfus | 33.32 | kJ/mol | Joback Method |
| hvap | 68.51 | kJ/mol | Joback Method |
| log10ws | -4.05 | | Crippen Method |
| logp | 3.265 | | Crippen Method |
| mcvol | 224.510 | ml/mol | McGowan Method |
| pc | 1772.85 | kPa | Joback Method |
| rinpol | 1855.00 | | NIST Webbook |
| rinpol | 1855.00 | | NIST Webbook |
| tb | 743.40 | K | Joback Method |
| tc | 937.13 | K | Joback Method |
| tf | 453.49 | K | Joback Method |
| vc | 0.871 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 646.98 | J/mol×K | 743.40 | Joback Method |
| cpg | 660.30 | J/mol×K | 775.69 | Joback Method |
| cpg | 672.71 | J/mol×K | 807.98 | Joback Method |
| cpg | 684.21 | J/mol×K | 840.26 | Joback Method |
| cpg | 694.83 | J/mol×K | 872.55 | Joback Method |
| cpg | 704.57 | J/mol×K | 904.84 | Joback Method |
| cpg | 713.47 | J/mol×K | 937.13 | Joback Method |

# Sources

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|---|---|
| **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=U391750&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |