# Glutaric acid, 4-(trifluoromethoxy)benzyl tridecyl ester

**Inchi:** InChI=1S/C26H39F3O5/c1-2-3-4-5-6-7-8-9-10-11-12-20-32-24(30)14-13-15-25(31)33-21
**InchiKey:** KPGJGJSUCGDRDI-UHFFFAOYSA-N
**Formula:** C26H39F3O5
**SMILES:** CCCCCCCCCCCCCOC(=O)CCCC(=O)OCc1ccc(OC(F)(F)F)cc1
**Mol. weight [g/mol]:** 488.58

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -883.61 | kJ/mol | Joback Method |
| hf | -1573.81 | kJ/mol | Joback Method |
| hfus | 65.34 | kJ/mol | Joback Method |
| hvap | 93.38 | kJ/mol | Joback Method |
| log10ws | -8.89 | | Crippen Method |
| logp | 7.653 | | Crippen Method |
| mcvol | 379.500 | ml/mol | McGowan Method |
| pc | 845.54 | kPa | Joback Method |
| rinpol | 2975.00 | | NIST Webbook |
| rinpol | 2975.00 | | NIST Webbook |
| tb | 995.52 | K | Joback Method |
| tc | 1224.52 | K | Joback Method |
| tf | 592.46 | K | Joback Method |
| vc | 1.492 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1293.29 | J/mol×K | 995.52 | Joback Method |
| cpg | 1310.02 | J/mol×K | 1033.69 | Joback Method |
| cpg | 1325.09 | J/mol×K | 1071.85 | Joback Method |
| cpg | 1338.57 | J/mol×K | 1110.02 | Joback Method |
| cpg | 1350.53 | J/mol×K | 1148.19 | Joback Method |
| cpg | 1361.03 | J/mol×K | 1186.35 | Joback Method |
| cpg | 1370.15 | J/mol×K | 1224.52 | 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=U377344&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 |