# Glutaric acid, monoamide, N-(3,5-di(trifluoromethyl)benzyl)-, tridecyl ester

**Inchi:** InChI=1S/C27H39F6NO3/c1-2-3-4-5-6-7-8-9-10-11-12-16-37-25(36)15-13-14-24(35)34-2
**InchiKey:** BUPGDKPBZNVDCX-UHFFFAOYSA-N
**Formula:** C27H39F6NO3
**SMILES:** CCCCCCCCCCCCCOC(=O)CCCC(=O)NCc1cc(C(F)(F)F)cc(C(F)(F)F)c1
**Mol. weight [g/mol]:** 539.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -1167.02 | kJ/mol | Joback Method |
| hf | -1885.09 | kJ/mol | Joback Method |
| hfus | 72.09 | kJ/mol | Joback Method |
| hvap | 94.14 | kJ/mol | Joback Method |
| log10ws | -9.92 | | Crippen Method |
| logp | 8.365 | | Crippen Method |
| mcvol | 397.140 | ml/mol | McGowan Method |
| pc | 763.52 | kPa | Joback Method |
| rinpol | 2970.00 | | NIST Webbook |
| tb | 1023.29 | K | Joback Method |
| tc | 1269.54 | K | Joback Method |
| tf | 628.64 | K | Joback Method |
| vc | 1.591 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1377.49 | J/mol×K | 1023.29 | Joback Method |
| cpg | 1395.72 | J/mol×K | 1064.33 | Joback Method |
| cpg | 1412.60 | J/mol×K | 1105.37 | Joback Method |
| cpg | 1428.28 | J/mol×K | 1146.42 | Joback Method |
| cpg | 1442.93 | J/mol×K | 1187.46 | Joback Method |
| cpg | 1456.71 | J/mol×K | 1228.50 | Joback Method |
| cpg | 1469.80 | J/mol×K | 1269.54 | 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=U360774&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |