# Glutaric acid, oct-1-en-3-yl tridec-2-yn-1-yl ester

**Inchi:** InChI=1S/C26H44O4/c1-4-7-9-10-11-12-13-14-15-16-18-23-29-25(27)21-19-22-26(28)30
**InchiKey:** MJANTWCMUQCFCG-UHFFFAOYSA-N
**Formula:** C26H44O4
**SMILES:** C=CC(CCCCC)OC(=O)CCCC(=O)OCC#CCCCCCCCCCC
**Mol. weight [g/mol]:** 420.63

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -11.60 | kJ/mol | Joback Method |
| hf | -677.12 | kJ/mol | Joback Method |
| hfus | 66.99 | kJ/mol | Joback Method |
| hvap | 92.88 | kJ/mol | Joback Method |
| log10ws | -8.19 | | Crippen Method |
| logp | 6.912 | | Crippen Method |
| mcvol | 379.180 | ml/mol | McGowan Method |
| pc | 858.98 | kPa | Joback Method |
| rinpol | 2840.00 | | NIST Webbook |
| rinpol | 2840.00 | | NIST Webbook |
| tb | 952.10 | K | Joback Method |
| tc | 1166.28 | K | Joback Method |
| tf | 616.44 | K | Joback Method |
| vc | 1.476 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1261.54 | J/mol×K | 952.10 | Joback Method |
| cpg | 1280.49 | J/mol×K | 987.80 | Joback Method |
| cpg | 1297.99 | J/mol×K | 1023.49 | Joback Method |
| cpg | 1314.07 | J/mol×K | 1059.19 | Joback Method |
| cpg | 1328.79 | J/mol×K | 1094.89 | Joback Method |
| cpg | 1342.18 | J/mol×K | 1130.58 | Joback Method |
| cpg | 1354.30 | J/mol×K | 1166.28 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U405358&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 |

# 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 |