# Glutaric acid, hex-4-yn-3-yl hexadecyl ester

**Inchi:** InChI=1S/C27H48O4/c1-4-7-8-9-10-11-12-13-14-15-16-17-18-19-24-30-26(28)22-20-23-
**InchiKey:** LCIWRDHFJUWLMB-UHFFFAOYSA-N
**Formula:** C27H48O4
**SMILES:** CC#CC(CC)OC(=O)CCCC(=O)OCCCCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 436.67

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -91.02 | kJ/mol | Joback Method |
| hf | -823.19 | kJ/mol | Joback Method |
| hfus | 70.86 | kJ/mol | Joback Method |
| hvap | 95.77 | kJ/mol | Joback Method |
| log10ws | -8.76 | | Crippen Method |
| logp | 7.526 | | Crippen Method |
| mcvol | 397.570 | ml/mol | McGowan Method |
| pc | 793.49 | kPa | Joback Method |
| rinpol | 3072.00 | | NIST Webbook |
| tb | 978.30 | K | Joback Method |
| tc | 1201.23 | K | Joback Method |
| tf | 629.47 | K | Joback Method |
| vc | 1.552 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1354.91 | J/mol×K | 978.30 | Joback Method |
| cpg | 1374.81 | J/mol×K | 1015.46 | Joback Method |
| cpg | 1393.05 | J/mol×K | 1052.61 | Joback Method |
| cpg | 1409.66 | J/mol×K | 1089.77 | Joback Method |
| cpg | 1424.69 | J/mol×K | 1126.92 | Joback Method |
| cpg | 1438.20 | J/mol×K | 1164.08 | Joback Method |
| cpg | 1450.23 | J/mol×K | 1201.23 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U359867&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

| | |
|---|---|
| **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 |

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