# Sebacic acid, ethyl tridec-2-ynyl ester

**Inchi:** InChI=1S/C25H44O4/c1-3-5-6-7-8-9-10-11-14-17-20-23-29-25(27)22-19-16-13-12-15-18
**InchiKey:** FIBLRJQDQILWQJ-UHFFFAOYSA-N
**Formula:** C25H44O4
**SMILES:** CCCCCCCCCCC#CCOC(=O)CCCCCCCCC(=O)OCC
**Mol. weight [g/mol]:** 408.61

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -105.42 | kJ/mol | Joback Method |
| hf | -776.63 | kJ/mol | Joback Method |
| hfus | 69.20 | kJ/mol | Joback Method |
| hvap | 91.71 | kJ/mol | Joback Method |
| log10ws | -7.81 | | Crippen Method |
| logp | 6.748 | | Crippen Method |
| mcvol | 369.390 | ml/mol | McGowan Method |
| pc | 882.62 | kPa | Joback Method |
| rinpol | 2904.00 | | NIST Webbook |
| tb | 932.98 | K | Joback Method |
| tc | 1142.70 | K | Joback Method |
| tf | 621.93 | K | Joback Method |
| vc | 1.446 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1227.56 | J/mol×K | 932.98 | Joback Method |
| cpg | 1246.71 | J/mol×K | 967.93 | Joback Method |
| cpg | 1264.43 | J/mol×K | 1002.89 | Joback Method |
| cpg | 1280.75 | J/mol×K | 1037.84 | Joback Method |
| cpg | 1295.72 | J/mol×K | 1072.80 | Joback Method |
| cpg | 1309.36 | J/mol×K | 1107.75 | Joback Method |
| cpg | 1321.71 | J/mol×K | 1142.70 | 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=U355854&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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