# Succinic acid, tridec-2-yn-1-yl 4-chloro-2-methoxyphenyl ester

**Inchi:** InChI=1S/C24H33ClO5/c1-3-4-5-6-7-8-9-10-11-12-13-18-29-23(26)16-17-24(27)30-21-15

**InchiKey:** HKXJGBRKJGJKKF-UHFFFAOYSA-N

**Formula:** C24H33ClO5

**SMILES:** CCCCCCCCCCC#CCOC(=O)CCC(=O)Oc1ccc(Cl)cc1OC

**Mol. weight [g/mol]:** 436.97

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -137.62 | kJ/mol | Joback Method |
| hf | -690.36 | kJ/mol | Joback Method |
| hfus | 65.26 | kJ/mol | Joback Method |
| hvap | 99.88 | kJ/mol | Joback Method |
| log10ws | -7.53 | | Crippen Method |
| logp | 6.112 | | Crippen Method |
| mcvol | 349.650 | ml/mol | McGowan Method |
| pc | 1094.27 | kPa | Joback Method |
| rinpol | 3214.00 | | NIST Webbook |
| rinpol | 3214.00 | | NIST Webbook |
| tb | 1006.59 | K | Joback Method |
| tc | 1232.90 | K | Joback Method |
| tf | 714.27 | K | Joback Method |
| vc | 1.349 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1116.14 | J/mol×K | 1006.59 | Joback Method |
| cpg | 1129.78 | J/mol×K | 1044.31 | Joback Method |
| cpg | 1141.83 | J/mol×K | 1082.03 | Joback Method |
| cpg | 1152.28 | J/mol×K | 1119.74 | Joback Method |
| cpg | 1161.18 | J/mol×K | 1157.46 | Joback Method |
| cpg | 1168.53 | J/mol×K | 1195.18 | Joback Method |
| cpg | 1174.34 | J/mol×K | 1232.90 | 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=U390947&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |