# Succinic acid, hept-2-yl dodec-9-yn-1-yl ester

**Inchi:** InChI=1S/C23H40O4/c1-4-6-8-9-10-11-12-13-14-16-20-26-22(24)18-19-23(25)27-21(3)1
**InchiKey:** CDDAOKDRPXJVMC-UHFFFAOYSA-N
**Formula:** C23H40O4
**SMILES:** CCC#CCCCCCCCCOC(=O)CCC(=O)OC(C)CCCCC
**Mol. weight [g/mol]:** 380.56

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -124.70 | kJ/mol | Joback Method |
| hf | -740.63 | kJ/mol | Joback Method |
| hfus | 60.50 | kJ/mol | Joback Method |
| hvap | 86.87 | kJ/mol | Joback Method |
| log10ws | -7.08 | | Crippen Method |
| logp | 5.966 | | Crippen Method |
| mcvol | 341.210 | ml/mol | McGowan Method |
| pc | 997.65 | kPa | Joback Method |
| rinpol | 2620.00 | | NIST Webbook |
| rinpol | 2620.00 | | NIST Webbook |
| tb | 886.78 | K | Joback Method |
| tc | 1086.62 | K | Joback Method |
| tf | 584.39 | K | Joback Method |
| vc | 1.327 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1102.99 | J/mol×K | 886.78 | Joback Method |
| cpg | 1121.36 | J/mol×K | 920.09 | Joback Method |
| cpg | 1138.48 | J/mol×K | 953.39 | Joback Method |
| cpg | 1154.37 | J/mol×K | 986.70 | Joback Method |
| cpg | 1169.05 | J/mol×K | 1020.00 | Joback Method |
| cpg | 1182.55 | J/mol×K | 1053.31 | Joback Method |
| cpg | 1194.89 | J/mol×K | 1086.62 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391000&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |