# Succinic acid, 2,4,6-trichlorophenyl pent-4-en-1-yl ester

**Inchi:** InChI=1S/C15H15Cl3O4/c1-2-3-4-7-21-13(19)5-6-14(20)22-15-11(17)8-10(16)9-12(15)18

**InchiKey:** CNDGHVKWCNDAKV-UHFFFAOYSA-N

**Formula:** C15H15Cl3O4

**SMILES:** C=CCCCOC(=O)CCC(=O)Oc1c(Cl)cc(Cl)cc1Cl

**Mol. weight [g/mol]:** 365.64

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -256.85 | kJ/mol | Joback Method |
| hf | -562.20 | kJ/mol | Joback Method |
| hfus | 44.36 | kJ/mol | Joback Method |
| hvap | 84.04 | kJ/mol | Joback Method |
| log10ws | -5.49 | | Crippen Method |
| logp | 4.842 | | Crippen Method |
| mcvol | 245.750 | ml/mol | McGowan Method |
| pc | 1812.32 | kPa | Joback Method |
| rinpol | 2392.00 | | NIST Webbook |
| rinpol | 2392.00 | | NIST Webbook |
| tb | 845.77 | K | Joback Method |
| tc | 1064.43 | K | Joback Method |
| tf | 555.11 | K | Joback Method |
| vc | 0.944 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 637.78 | J/mol×K | 845.77 | Joback Method |
| cpg | 648.53 | J/mol×K | 882.21 | Joback Method |
| cpg | 658.34 | J/mol×K | 918.66 | Joback Method |
| cpg | 667.22 | J/mol×K | 955.10 | Joback Method |
| cpg | 675.17 | J/mol×K | 991.54 | Joback Method |
| cpg | 682.21 | J/mol×K | 1027.99 | Joback Method |
| cpg | 688.35 | J/mol×K | 1064.43 | Joback Method |
| dvisc | 0.0004420 | Pa×s | 555.11 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002954 | Pa×s | 603.55 | Joback Method |
| dvisc | 0.0002096 | Pa×s | 652.00 | Joback Method |
| dvisc | 0.0001559 | Pa×s | 700.44 | Joback Method |
| dvisc | 0.0001205 | Pa×s | 748.88 | Joback Method |
| dvisc | 0.0000961 | Pa×s | 797.33 | Joback Method |
| dvisc | 0.0000787 | Pa×s | 845.77 | Joback Method |

# Sources

| | |
|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U391076&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 |
| **dvisc:** | Dynamic viscosity |
| **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 |