# Sebacic acid, 3-chlorophenyl octyl ester

**Inchi:** InChI=1S/C24H37ClO4/c1-2-3-4-5-10-13-19-28-23(26)17-11-8-6-7-9-12-18-24(27)29-22-
**InchiKey:** AUPBFYHUWSLFTP-UHFFFAOYSA-N
**Formula:** C24H37ClO4
**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1cccc(Cl)c1
**Mol. weight [g/mol]:** 425.00

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -225.79 | kJ/mol | Joback Method |
| hf | -818.97 | kJ/mol | Joback Method |
| hfus | 61.34 | kJ/mol | Joback Method |
| hvap | 94.65 | kJ/mol | Joback Method |
| log10ws | -8.03 | | Crippen Method |
| logp | 7.270 | | Crippen Method |
| mcvol | 352.380 | ml/mol | McGowan Method |
| pc | 1007.17 | kPa | Joback Method |
| rinpol | 3172.00 | | NIST Webbook |
| tb | 970.19 | K | Joback Method |
| tc | 1187.80 | K | Joback Method |
| tf | 573.42 | K | Joback Method |
| vc | 1.369 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1146.11 | J/mol×K | 970.19 | Joback Method |
| cpg | 1161.98 | J/mol×K | 1006.46 | Joback Method |
| cpg | 1176.44 | J/mol×K | 1042.73 | Joback Method |
| cpg | 1189.54 | J/mol×K | 1079.00 | Joback Method |
| cpg | 1201.32 | J/mol×K | 1115.26 | Joback Method |
| cpg | 1211.83 | J/mol×K | 1151.53 | Joback Method |
| cpg | 1221.10 | J/mol×K | 1187.80 | Joback Method |
| dvisc | 0.0003068 | Pa×s | 573.42 | Joback Method |
| dvisc | 0.0001644 | Pa×s | 639.55 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000990 | Pa×s | 705.68 | Joback Method |
| dvisc | 0.0000650 | Pa×s | 771.81 | Joback Method |
| dvisc | 0.0000457 | Pa×s | 837.93 | Joback Method |
| dvisc | 0.0000338 | Pa×s | 904.06 | Joback Method |
| dvisc | 0.0000260 | Pa×s | 970.19 | Joback Method |

# Sources

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|---|---|
| **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=U354864&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# Legend

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