# Sebacic acid, 2,6-dichlorophenyl octyl ester

**Inchi:** InChI=1S/C24H36Cl2O4/c1-2-3-4-5-10-13-19-29-22(27)17-11-8-6-7-9-12-18-23(28)30-24
**InchiKey:** DVWZKZUDWZTVND-UHFFFAOYSA-N
**Formula:** C24H36Cl2O4
**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1c(Cl)cccc1Cl
**Mol. weight [g/mol]:** 459.45

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -247.35 | kJ/mol | Joback Method |
| hf | -846.18 | kJ/mol | Joback Method |
| hfus | 65.15 | kJ/mol | Joback Method |
| hvap | 99.70 | kJ/mol | Joback Method |
| log10ws | -8.72 | | Crippen Method |
| logp | 7.923 | | Crippen Method |
| mcvol | 364.620 | ml/mol | McGowan Method |
| pc | 974.73 | kPa | Joback Method |
| rinpol | 3309.00 | | NIST Webbook |
| rinpol | 3309.00 | | NIST Webbook |
| tb | 1012.60 | K | Joback Method |
| tc | 1239.97 | K | Joback Method |
| tf | 615.86 | K | Joback Method |
| vc | 1.417 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1169.66 | J/mol×K | 1012.60 | Joback Method |
| cpg | 1184.22 | J/mol×K | 1050.50 | Joback Method |
| cpg | 1197.29 | J/mol×K | 1088.39 | Joback Method |
| cpg | 1208.93 | J/mol×K | 1126.29 | Joback Method |
| cpg | 1219.16 | J/mol×K | 1164.18 | Joback Method |
| cpg | 1228.05 | J/mol×K | 1202.08 | Joback Method |
| cpg | 1235.63 | J/mol×K | 1239.97 | Joback Method |
| dvisc | 0.0002177 | Pa×s | 615.86 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001239 | Pa×s | 681.98 | Joback Method |
| dvisc | 0.0000779 | Pa×s | 748.11 | Joback Method |
| dvisc | 0.0000528 | Pa×s | 814.23 | Joback Method |
| dvisc | 0.0000380 | Pa×s | 880.35 | Joback Method |
| dvisc | 0.0000286 | Pa×s | 946.48 | Joback Method |
| dvisc | 0.0000223 | Pa×s | 1012.60 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U354879&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

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