# Sebacic acid, 4-chloro-2-methylphenyl octyl ester

**Inchi:** InChI=1S/C25H39ClO4/c1-3-4-5-6-11-14-19-29-24(27)15-12-9-7-8-10-13-16-25(28)30-23

**InchiKey:** QJHNGQYICWBFEO-UHFFFAOYSA-N

**Formula:** C25H39ClO4

**SMILES:** CCCCCCCCOC(=O)CCCCCCCCC(=O)Oc1ccc(Cl)cc1C

**Mol. weight [g/mol]:** 439.03

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -227.00 | kJ/mol | Joback Method |
| hf | -851.08 | kJ/mol | Joback Method |
| hfus | 63.54 | kJ/mol | Joback Method |
| hvap | 97.54 | kJ/mol | Joback Method |
| log10ws | -8.51 | | Crippen Method |
| logp | 7.578 | | Crippen Method |
| mcvol | 366.470 | ml/mol | McGowan Method |
| pc | 939.79 | kPa | Joback Method |
| rinpol | 3206.00 | | NIST Webbook |
| rinpol | 3206.00 | | NIST Webbook |
| tb | 998.05 | K | Joback Method |
| tc | 1222.32 | K | Joback Method |
| tf | 597.21 | K | Joback Method |
| vc | 1.425 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1206.93 | J/mol×K | 998.05 | Joback Method |
| cpg | 1272.01 | J/mol×K | 1184.94 | Joback Method |
| cpg | 1261.89 | J/mol×K | 1147.56 | Joback Method |
| cpg | 1250.36 | J/mol×K | 1110.18 | Joback Method |
| cpg | 1237.39 | J/mol×K | 1072.81 | Joback Method |
| cpg | 1222.93 | J/mol×K | 1035.43 | Joback Method |
| cpg | 1280.79 | J/mol×K | 1222.32 | Joback Method |
| dvisc | 0.0000229 | Pa×s | 998.05 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000294 | Pa×s | 931.24 | Joback Method |
| dvisc | 0.0000393 | Pa×s | 864.44 | Joback Method |
| dvisc | 0.0000552 | Pa×s | 797.63 | Joback Method |
| dvisc | 0.0000825 | Pa×s | 730.82 | Joback Method |
| dvisc | 0.0001336 | Pa×s | 664.02 | Joback Method |
| dvisc | 0.0002411 | Pa×s | 597.21 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U355106&Units=SI |

# 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 |

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