# Sebacic acid, di(4-methylpent-2-yl) ester

**Inchi:** InChI=1S/C22H42O4/c1-17(2)15-19(5)25-21(23)13-11-9-7-8-10-12-14-22(24)26-20(6)16
**InchiKey:** DPKYGJASYLZPAZ-UHFFFAOYSA-N
**Formula:** C22H42O4
**SMILES:** CC(C)CC(C)OC(=O)CCCCCCCCC(=O)OC(C)CC(C)C
**Mol. weight [g/mol]:** 370.57

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -343.24 | kJ/mol | Joback Method |
| hf | -1008.13 | kJ/mol | Joback Method |
| hfus | 44.22 | kJ/mol | Joback Method |
| hvap | 81.33 | kJ/mol | Joback Method |
| log10ws | -6.50 | | Crippen Method |
| logp | 6.063 | | Crippen Method |
| mcvol | 335.720 | ml/mol | McGowan Method |
| pc | 972.91 | kPa | Joback Method |
| rinpol | 2320.00 | | NIST Webbook |
| rinpol | 2320.00 | | NIST Webbook |
| tb | 853.58 | K | Joback Method |
| tc | 1046.48 | K | Joback Method |
| tf | 422.02 | K | Joback Method |
| vc | 1.292 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1093.89 | J/mol×K | 853.58 | Joback Method |
| cpg | 1113.12 | J/mol×K | 885.73 | Joback Method |
| cpg | 1131.10 | J/mol×K | 917.88 | Joback Method |
| cpg | 1147.86 | J/mol×K | 950.03 | Joback Method |
| cpg | 1163.41 | J/mol×K | 982.18 | Joback Method |
| cpg | 1177.78 | J/mol×K | 1014.33 | Joback Method |
| cpg | 1191.00 | J/mol×K | 1046.48 | Joback Method |
| dvisc | 0.0014060 | Pa×s | 422.02 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0004550 | Pa×s | 493.95 | Joback Method |
| dvisc | 0.0001962 | Pa×s | 565.87 | Joback Method |
| dvisc | 0.0001022 | Pa×s | 637.80 | Joback Method |
| dvisc | 0.0000608 | Pa×s | 709.73 | Joback Method |
| dvisc | 0.0000398 | Pa×s | 781.65 | Joback Method |
| dvisc | 0.0000280 | Pa×s | 853.58 | Joback Method |

# Sources

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|---|---|
| **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=U355364&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 |