# Adipic acid, decyl 3-heptyl ester

**Inchi:** InChI=1S/C23H44O4/c1-4-7-9-10-11-12-13-16-20-26-22(24)18-14-15-19-23(25)27-21(6-
**InchiKey:** HVXZBADBKNOWAQ-UHFFFAOYSA-N
**Formula:** C23H44O4
**SMILES:** CCCCCCCCCCOC(=O)CCCCC(=O)OC(CC)CCCC
**Mol. weight [g/mol]:** 384.59

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -327.50 | kJ/mol | Joback Method |
| hf | -1012.93 | kJ/mol | Joback Method |
| hfus | 57.38 | kJ/mol | Joback Method |
| hvap | 84.72 | kJ/mol | Joback Method |
| log10ws | -7.29 | | Crippen Method |
| logp | 6.743 | | Crippen Method |
| mcvol | 349.810 | ml/mol | McGowan Method |
| pc | 903.97 | kPa | Joback Method |
| rinpol | 2520.00 | | NIST Webbook |
| tb | 877.78 | K | Joback Method |
| tc | 1074.72 | K | Joback Method |
| tf | 478.29 | K | Joback Method |
| vc | 1.365 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1154.96 | J/mol×K | 877.78 | Joback Method |
| cpg | 1174.58 | J/mol×K | 910.60 | Joback Method |
| cpg | 1192.90 | J/mol×K | 943.43 | Joback Method |
| cpg | 1209.94 | J/mol×K | 976.25 | Joback Method |
| cpg | 1225.74 | J/mol×K | 1009.07 | Joback Method |
| cpg | 1240.32 | J/mol×K | 1041.89 | Joback Method |
| cpg | 1253.72 | J/mol×K | 1074.72 | Joback Method |
| dvisc | 0.0006901 | Pa×s | 478.29 | Joback Method |
| dvisc | 0.0003008 | Pa×s | 544.87 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001571 | Pa×s | 611.45 | Joback Method |
| dvisc | 0.0000932 | Pa×s | 678.03 | Joback Method |
| dvisc | 0.0000607 | Pa×s | 744.62 | Joback Method |
| dvisc | 0.0000424 | Pa×s | 811.20 | Joback Method |
| dvisc | 0.0000313 | Pa×s | 877.78 | Joback Method |

# Sources

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|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U353655&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

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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 |