# Adipic acid, ethyl pent-4-en-2-yl ester

**Inchi:** InChI=1S/C13H22O4/c1-4-8-11(3)17-13(15)10-7-6-9-12(14)16-5-2/h4,11H,1,5-10H2,2-3H
**InchiKey:** DKCALIPCOLFPSF-UHFFFAOYSA-N
**Formula:** C13H22O4
**SMILES:** C=CCC(C)OC(=O)CCCCC(=O)OCC
**Mol. weight [g/mol]:** 242.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -323.86 | kJ/mol | Joback Method |
| hf | -681.10 | kJ/mol | Joback Method |
| hfus | 30.20 | kJ/mol | Joback Method |
| hvap | 61.79 | kJ/mol | Joback Method |
| log10ws | -2.95 | | Crippen Method |
| logp | 2.618 | | Crippen Method |
| mcvol | 204.610 | ml/mol | McGowan Method |
| pc | 1851.52 | kPa | Joback Method |
| rinpol | 1573.00 | | NIST Webbook |
| tb | 645.66 | K | Joback Method |
| tc | 827.30 | K | Joback Method |
| tf | 363.83 | K | Joback Method |
| vc | 0.786 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 546.28 | J/mol×K | 645.66 | Joback Method |
| cpg | 613.53 | J/mol×K | 797.03 | Joback Method |
| cpg | 601.47 | J/mol×K | 766.76 | Joback Method |
| cpg | 588.71 | J/mol×K | 736.48 | Joback Method |
| cpg | 575.27 | J/mol×K | 706.21 | Joback Method |
| cpg | 561.13 | J/mol×K | 675.93 | Joback Method |
| cpg | 624.91 | J/mol×K | 827.30 | Joback Method |
| dvisc | 0.0001317 | Pa×s | 645.66 | Joback Method |
| dvisc | 0.0001730 | Pa×s | 598.69 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002381 | Pa×s | 551.72 | Joback Method |
| dvisc | 0.0003476 | Pa×s | 504.75 | Joback Method |
| dvisc | 0.0005485 | Pa×s | 457.77 | Joback Method |
| dvisc | 0.0009606 | Pa×s | 410.80 | Joback Method |
| dvisc | 0.0019445 | Pa×s | 363.83 | 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=U354117&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 |