# Adipic acid, eicosyl pent-4-enyl ester

**Inchi:** InChI=1S/C31H58O4/c1-3-5-7-8-9-10-11-12-13-14-15-16-17-18-19-20-21-25-29-35-31(3
**InchiKey:** QCHFTUDVGAHNJF-UHFFFAOYSA-N
**Formula:** C31H58O4
**SMILES:** C=CCCCOC(=O)CCCCC(=O)OCCCCCCCCCCCCCCCCCCCC
**Mol. weight [g/mol]:** 494.79

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -169.86 | kJ/mol | Joback Method |
| hf | -1047.34 | kJ/mol | Joback Method |
| hfus | 80.34 | kJ/mol | Joback Method |
| hvap | 102.24 | kJ/mol | Joback Method |
| log10ws | -10.38 | | Crippen Method |
| logp | 9.641 | | Crippen Method |
| mcvol | 458.230 | ml/mol | McGowan Method |
| pc | 606.66 | kPa | Joback Method |
| rinpol | 3433.00 | | NIST Webbook |
| tb | 1057.94 | K | Joback Method |
| tc | 1335.41 | K | Joback Method |
| tf | 581.69 | K | Joback Method |
| vc | 1.800 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 1639.81 | J/mol×K | 1057.94 | Joback Method |
| cpg | 1664.34 | J/mol×K | 1104.19 | Joback Method |
| cpg | 1686.29 | J/mol×K | 1150.43 | Joback Method |
| cpg | 1705.79 | J/mol×K | 1196.68 | Joback Method |
| cpg | 1722.98 | J/mol×K | 1242.92 | Joback Method |
| cpg | 1738.03 | J/mol×K | 1289.17 | Joback Method |
| cpg | 1751.06 | J/mol×K | 1335.41 | Joback Method |
| dvisc | 0.0002165 | Pa×s | 581.69 | Joback Method |
| dvisc | 0.0000968 | Pa×s | 661.07 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0000514 | Pa×s | 740.44 | Joback Method |
| dvisc | 0.0000309 | Pa×s | 819.82 | Joback Method |
| dvisc | 0.0000203 | Pa×s | 899.19 | Joback Method |
| dvisc | 0.0000143 | Pa×s | 978.57 | Joback Method |
| dvisc | 0.0000106 | Pa×s | 1057.94 | 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=U353808&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 |

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