# Adipic acid, 2,2-dichloroethyl undecyl ester

**Inchi:** InChI=1S/C19H34Cl2O4/c1-2-3-4-5-6-7-8-9-12-15-24-18(22)13-10-11-14-19(23)25-16-17
**InchiKey:** FASBMBQSXCTYIH-UHFFFAOYSA-N
**Formula:** C19H34Cl2O4
**SMILES:** CCCCCCCCCCCOC(=O)CCCCC(=O)OCC(Cl)Cl
**Mol. weight [g/mol]:** 397.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -385.04 | kJ/mol | Joback Method |
| hf | -961.85 | kJ/mol | Joback Method |
| hfus | 55.41 | kJ/mol | Joback Method |
| hvap | 84.58 | kJ/mol | Joback Method |
| log10ws | -6.41 | | Crippen Method |
| logp | 5.968 | | Crippen Method |
| mcvol | 317.930 | ml/mol | McGowan Method |
| pc | 1099.35 | kPa | Joback Method |
| rinpol | 2599.00 | | NIST Webbook |
| rinpol | 2599.00 | | NIST Webbook |
| tb | 861.12 | K | Joback Method |
| tc | 1056.11 | K | Joback Method |
| tf | 493.05 | K | Joback Method |
| vc | 1.240 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 970.57 | J/mol×K | 861.12 | Joback Method |
| cpg | 986.62 | J/mol×K | 893.62 | Joback Method |
| cpg | 1001.58 | J/mol×K | 926.12 | Joback Method |
| cpg | 1015.48 | J/mol×K | 958.61 | Joback Method |
| cpg | 1028.34 | J/mol×K | 991.11 | Joback Method |
| cpg | 1040.18 | J/mol×K | 1023.61 | Joback Method |
| cpg | 1051.01 | J/mol×K | 1056.11 | Joback Method |
| dvisc | 0.0006685 | Pa×s | 493.05 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0003248 | Pa×s | 554.39 | Joback Method |
| dvisc | 0.0001822 | Pa×s | 615.74 | Joback Method |
| dvisc | 0.0001135 | Pa×s | 677.09 | Joback Method |
| dvisc | 0.0000765 | Pa×s | 738.43 | Joback Method |
| dvisc | 0.0000548 | Pa×s | 799.77 | Joback Method |
| dvisc | 0.0000411 | Pa×s | 861.12 | Joback Method |

# Sources

**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=U353585&Units=SI
**Crippen Method:** http://pubs.acs.org/doi/abs/10.1021/ci990307l

# 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