# Adipic acid, 2-decyl propyl ester

**Inchi:** InChI=1S/C19H36O4/c1-4-6-7-8-9-10-13-17(3)23-19(21)15-12-11-14-18(20)22-16-5-2/h1
**InchiKey:** ZGJGSSALJYFBPE-UHFFFAOYSA-N
**Formula:** C19H36O4
**SMILES:** CCCCCCCCC(C)OC(=O)CCCCC(=O)OCCC
**Mol. weight [g/mol]:** 328.49

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -361.18 | kJ/mol | Joback Method |
| hf | -930.37 | kJ/mol | Joback Method |
| hfus | 47.02 | kJ/mol | Joback Method |
| hvap | 75.81 | kJ/mol | Joback Method |
| log10ws | -5.61 | | Crippen Method |
| logp | 5.182 | | Crippen Method |
| mcvol | 293.450 | ml/mol | McGowan Method |
| pc | 1155.35 | kPa | Joback Method |
| rinpol | 2151.00 | | NIST Webbook |
| tb | 786.26 | K | Joback Method |
| tc | 968.16 | K | Joback Method |
| tf | 433.21 | K | Joback Method |
| vc | 1.141 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 909.39 | J/mol×K | 786.26 | Joback Method |
| cpg | 927.32 | J/mol×K | 816.58 | Joback Method |
| cpg | 944.26 | J/mol×K | 846.89 | Joback Method |
| cpg | 960.22 | J/mol×K | 877.21 | Joback Method |
| cpg | 975.21 | J/mol×K | 907.53 | Joback Method |
| cpg | 989.26 | J/mol×K | 937.85 | Joback Method |
| cpg | 1002.36 | J/mol×K | 968.16 | Joback Method |
| dvisc | 0.0011109 | Pa×s | 433.21 | Joback Method |
| dvisc | 0.0005025 | Pa×s | 492.05 | Joback Method |

| | | | | |
|---|---|---|---|---|
| dvisc | 0.0002693 | Pa×s | 550.89 | Joback Method |
| dvisc | 0.0001628 | Pa×s | 609.74 | Joback Method |
| dvisc | 0.0001075 | Pa×s | 668.58 | Joback Method |
| dvisc | 0.0000759 | Pa×s | 727.42 | Joback Method |
| dvisc | 0.0000565 | Pa×s | 786.26 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U353595&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

| | |
|---|---|
| **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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