# Adipic acid, 2,4-dimethylpent-3-yl heptyl ester

**Inchi:** InChI=1S/C20H38O4/c1-6-7-8-9-12-15-23-18(21)13-10-11-14-19(22)24-20(16(2)3)17(4)5
**InchiKey:** BGFMQQJKGVEIFK-UHFFFAOYSA-N
**Formula:** C20H38O4
**SMILES:** CCCCCCCOC(=O)CCCCC(=O)OC(C(C)C)C(C)C
**Mol. weight [g/mol]:** 342.51

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -357.64 | kJ/mol | Joback Method |
| hf | -961.57 | kJ/mol | Joback Method |
| hfus | 42.56 | kJ/mol | Joback Method |
| hvap | 77.26 | kJ/mol | Joback Method |
| log10ws | -5.55 | | Crippen Method |
| logp | 5.284 | | Crippen Method |
| mcvol | 307.540 | ml/mol | McGowan Method |
| pc | 1094.99 | kPa | Joback Method |
| rinpol | 2189.00 | | NIST Webbook |
| tb | 808.26 | K | Joback Method |
| tc | 994.56 | K | Joback Method |
| tf | 414.48 | K | Joback Method |
| vc | 1.185 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 970.62 | J/mol×K | 808.26 | Joback Method |
| cpg | 989.13 | J/mol×K | 839.31 | Joback Method |
| cpg | 1006.54 | J/mol×K | 870.36 | Joback Method |
| cpg | 1022.88 | J/mol×K | 901.41 | Joback Method |
| cpg | 1038.15 | J/mol×K | 932.46 | Joback Method |
| cpg | 1052.38 | J/mol×K | 963.51 | Joback Method |
| cpg | 1065.59 | J/mol×K | 994.56 | Joback Method |
| dvisc | 0.0014761 | Pa×s | 414.48 | Joback Method |
| dvisc | 0.0005410 | Pa×s | 480.11 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0002524 | Pa×s | 545.74 | Joback Method |
| dvisc | 0.0001387 | Pa×s | 611.37 | Joback Method |
| dvisc | 0.0000856 | Pa×s | 677.00 | Joback Method |
| dvisc | 0.0000575 | Pa×s | 742.63 | Joback Method |
| dvisc | 0.0000412 | Pa×s | 808.26 | 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=U353524&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 |