# Adipic acid, hexyl 2,3,6-trichlorophenyl ester

**Inchi:** InChI=1S/C18H23Cl3O4/c1-2-3-4-7-12-24-15(22)8-5-6-9-16(23)25-18-14(20)11-10-13(19
**InchiKey:** NAPOBLWQTBMNMI-UHFFFAOYSA-N
**Formula:** C18H23Cl3O4
**SMILES:** CCCCCCOC(=O)CCCCC(=O)Oc1c(Cl)ccc(Cl)c1Cl
**Mol. weight [g/mol]:** 409.73

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -319.43 | kJ/mol | Joback Method |
| hf | -749.55 | kJ/mol | Joback Method |
| hfus | 53.41 | kJ/mol | Joback Method |
| hvap | 91.39 | kJ/mol | Joback Method |
| log10ws | -6.89 | | Crippen Method |
| logp | 6.236 | | Crippen Method |
| mcvol | 292.320 | ml/mol | McGowan Method |
| pc | 1393.33 | kPa | Joback Method |
| rinpol | 2743.00 | | NIST Webbook |
| tb | 917.73 | K | Joback Method |
| tc | 1133.26 | K | Joback Method |
| tf | 590.68 | K | Joback Method |
| vc | 1.131 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 834.27 | J/mol×K | 917.73 | Joback Method |
| cpg | 883.34 | J/mol×K | 1097.33 | Joback Method |
| cpg | 875.72 | J/mol×K | 1061.41 | Joback Method |
| cpg | 867.01 | J/mol×K | 1025.49 | Joback Method |
| cpg | 857.21 | J/mol×K | 989.57 | Joback Method |
| cpg | 846.30 | J/mol×K | 953.65 | Joback Method |
| cpg | 889.90 | J/mol×K | 1133.26 | Joback Method |
| dvisc | 0.0000477 | Pa×s | 917.73 | Joback Method |
| dvisc | 0.0000592 | Pa×s | 863.22 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000757 | Pa×s | 808.71 | Joback Method |
| dvisc | 0.0001001 | Pa×s | 754.21 | Joback Method |
| dvisc | 0.0001384 | Pa×s | 699.70 | Joback Method |
| dvisc | 0.0002021 | Pa×s | 645.19 | Joback Method |
| dvisc | 0.0003165 | Pa×s | 590.68 | 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=U353937&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 |