# 1,2,4,5-Benzene-tetracarboxylic acid, dipropyl ester

**Inchi:** InChI=1S/C16H18O8/c1-3-5-23-15(21)11-7-10(14(19)20)12(8-9(11)13(17)18)16(22)24-6
**InchiKey:** UMPAINQRYDYVBA-UHFFFAOYSA-N
**Formula:** C16H18O8
**SMILES:** CCCOC(=O)c1cc(C(=O)O)c(C(=O)OCCC)cc1C(=O)O
**Mol. weight [g/mol]:** 338.31
**CAS:** 56941-72-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| chs | -7224.40 ± 2.30 | kJ/mol | NIST Webbook |
| gf | -831.96 | kJ/mol | Joback Method |
| hf | -1190.67 | kJ/mol | Joback Method |
| hfs | -1644.20 ± 2.60 | kJ/mol | NIST Webbook |
| hfus | 47.02 | kJ/mol | Joback Method |
| hvap | 120.63 | kJ/mol | Joback Method |
| log10ws | -3.75 | | Crippen Method |
| logp | 2.217 | | Crippen Method |
| mcvol | 242.300 | ml/mol | McGowan Method |
| pc | 2342.82 | kPa | Joback Method |
| tb | 1051.78 | K | Joback Method |
| tc | 1288.97 | K | Joback Method |
| tf | 699.88 | K | Joback Method |
| vc | 0.921 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 758.12 | J/mol×K | 1051.78 | Joback Method |
| cpg | 764.63 | J/mol×K | 1091.31 | Joback Method |
| cpg | 769.81 | J/mol×K | 1130.84 | Joback Method |
| cpg | 773.65 | J/mol×K | 1170.38 | Joback Method |
| cpg | 776.16 | J/mol×K | 1209.91 | Joback Method |
| cpg | 777.33 | J/mol×K | 1249.44 | Joback Method |
| cpg | 777.18 | J/mol×K | 1288.97 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000259 | Pa×s | 699.88 | Joback Method |
| dvisc | 0.0000128 | Pa×s | 758.53 | Joback Method |
| dvisc | 0.0000070 | Pa×s | 817.18 | Joback Method |
| dvisc | 0.0000042 | Pa×s | 875.83 | Joback Method |
| dvisc | 0.0000026 | Pa×s | 934.48 | Joback Method |
| dvisc | 0.0000018 | Pa×s | 993.13 | Joback Method |
| dvisc | 0.0000012 | Pa×s | 1051.78 | Joback Method |

# Sources

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|---|---|
| **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=C56941721&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

| | |
|---|---|
| **chs:** | Standard solid enthalpy of combustion |
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **gf:** | Standard Gibbs free energy of formation |
| **hf:** | Enthalpy of formation at standard conditions |
| **hfs:** | Solid phase 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |

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