# (4-pentoxy-phenyl)-acetic acid, methyl ester

**Inchi:** InChI=1S/C14H20O3/c1-3-4-5-10-17-13-8-6-12(7-9-13)11-14(15)16-2/h6-9H,3-5,10-11H
**InchiKey:** DGBCBOUXLPQBRT-UHFFFAOYSA-N
**Formula:** C14H20O3
**SMILES:** CCCCCOc1ccc(CC(=O)OC)cc1
**Mol. weight [g/mol]:** 236.31

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -169.14 | kJ/mol | Joback Method |
| hf | -484.25 | kJ/mol | Joback Method |
| hfus | 29.64 | kJ/mol | Joback Method |
| hvap | 61.26 | kJ/mol | Joback Method |
| log10ws | -3.35 | | Crippen Method |
| logp | 2.971 | | Crippen Method |
| mcvol | 197.670 | ml/mol | McGowan Method |
| pc | 2034.55 | kPa | Joback Method |
| rinpol | 1770.00 | | NIST Webbook |
| rinpol | 1770.00 | | NIST Webbook |
| tb | 650.09 | K | Joback Method |
| tc | 849.38 | K | Joback Method |
| tf | 380.87 | K | Joback Method |
| vc | 0.753 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 521.01 | J/mol×K | 650.09 | Joback Method |
| cpg | 591.63 | J/mol×K | 816.17 | Joback Method |
| cpg | 579.17 | J/mol×K | 782.95 | Joback Method |
| cpg | 565.89 | J/mol×K | 749.74 | Joback Method |
| cpg | 551.77 | J/mol×K | 716.52 | Joback Method |
| cpg | 536.82 | J/mol×K | 683.31 | Joback Method |
| cpg | 603.27 | J/mol×K | 849.38 | Joback Method |
| dvisc | 0.0001181 | Pa×s | 650.09 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0001501 | Pa×s | 605.22 | Joback Method |
| dvisc | 0.0001982 | Pa×s | 560.35 | Joback Method |
| dvisc | 0.0002748 | Pa×s | 515.48 | Joback Method |
| dvisc | 0.0004053 | Pa×s | 470.61 | Joback Method |
| dvisc | 0.0006488 | Pa×s | 425.74 | Joback Method |
| dvisc | 0.0011604 | Pa×s | 380.87 | Joback Method |

# Sources

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|---|---|
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R158115&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 |

# 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 |