# l-Methionine, N-(p-toluoyl)-, methyl ester

**Inchi:** InChI=1S/C14H19NO3S/c1-10-4-6-11(7-5-10)13(16)15-12(8-9-19-3)14(17)18-2/h4-7,12H
**InchiKey:** QMWSBWKFWFGDFP-UHFFFAOYSA-N
**Formula:** C14H19NO3S
**SMILES:** COC(=O)C(CCSC)NC(=O)c1ccc(C)cc1
**Mol. weight [g/mol]:** 281.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -72.99 | kJ/mol | Joback Method |
| hf | -374.55 | kJ/mol | Joback Method |
| hfus | 35.76 | kJ/mol | Joback Method |
| hvap | 78.46 | kJ/mol | Joback Method |
| log10ws | -3.24 | | Crippen Method |
| logp | 2.020 | | Crippen Method |
| mcvol | 219.700 | ml/mol | McGowan Method |
| pc | 2269.73 | kPa | Joback Method |
| rinpol | 2245.00 | | NIST Webbook |
| rinpol | 2245.00 | | NIST Webbook |
| tb | 800.05 | K | Joback Method |
| tc | 1024.98 | K | Joback Method |
| tf | 480.63 | K | Joback Method |
| vc | 0.825 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 621.54 | J/mol×K | 800.05 | Joback Method |
| cpg | 635.00 | J/mol×K | 837.54 | Joback Method |
| cpg | 647.34 | J/mol×K | 875.03 | Joback Method |
| cpg | 658.57 | J/mol×K | 912.51 | Joback Method |
| cpg | 668.71 | J/mol×K | 950.00 | Joback Method |
| cpg | 677.79 | J/mol×K | 987.49 | Joback Method |
| cpg | 685.83 | J/mol×K | 1024.98 | 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=U299648&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# Legend

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|---|---|
| **cpg:** | Ideal gas heat capacity |
| **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 |