# 1-Adamantanecarboxamide, N-(4-methoxyphenyl)-

**Inchi:** InChI=1S/C18H23NO2/c1-21-16-4-2-15(3-5-16)19-17(20)18-9-12-6-13(10-18)8-14(7-12)
**InchiKey:** DOMQVXNITFPQNL-UHFFFAOYSA-N
**Formula:** C18H23NO2
**SMILES:** COc1ccc(NC(=O)C23CC4CC(CC(C4)C2)C3)cc1
**Mol. weight [g/mol]:** 285.38

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 215.88 | kJ/mol | Joback Method |
| hf | -173.98 | kJ/mol | Joback Method |
| hfus | 30.99 | kJ/mol | Joback Method |
| hvap | 72.64 | kJ/mol | Joback Method |
| log10ws | -4.28 | | Crippen Method |
| logp | 3.850 | | Crippen Method |
| mcvol | 225.560 | ml/mol | McGowan Method |
| pc | 2175.46 | kPa | Joback Method |
| tb | 789.42 | K | Joback Method |
| tc | 1028.47 | K | Joback Method |
| tf | 526.34 | K | Joback Method |
| vc | 0.855 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 725.64 | J/mol×K | 789.42 | Joback Method |
| cpg | 745.46 | J/mol×K | 829.26 | Joback Method |
| cpg | 764.58 | J/mol×K | 869.10 | Joback Method |
| cpg | 783.28 | J/mol×K | 908.95 | Joback Method |
| cpg | 801.81 | J/mol×K | 948.79 | Joback Method |
| cpg | 820.42 | J/mol×K | 988.63 | Joback Method |
| cpg | 839.39 | J/mol×K | 1028.47 | Joback Method |

# Sources

| | |
|---|---|
| **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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307468&Units=SI |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |