# Acetamide, N-(3-methylphenyl)-2-methoxy-

**Inchi:** InChI=1S/C10H13NO2/c1-8-4-3-5-9(6-8)11-10(12)7-13-2/h3-6H,7H2,1-2H3,(H,11,12)
**InchiKey:** KHVUHFOOPAOLHJ-UHFFFAOYSA-N
**Formula:** C10H13NO2
**SMILES:** COCC(=O)Nc1cccc(C)c1
**Mol. weight [g/mol]:** 179.22

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -8.43 | kJ/mol | Joback Method |
| hf | -216.00 | kJ/mol | Joback Method |
| hfus | 23.19 | kJ/mol | Joback Method |
| hvap | 56.38 | kJ/mol | Joback Method |
| log10ws | -1.66 | | Crippen Method |
| logp | 1.580 | | Crippen Method |
| mcvol | 145.420 | ml/mol | McGowan Method |
| pc | 3076.16 | kPa | Joback Method |
| rinpol | 1554.00 | | NIST Webbook |
| tb | 586.32 | K | Joback Method |
| tc | 800.02 | K | Joback Method |
| tf | 366.22 | K | Joback Method |
| vc | 0.546 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 347.62 | J/mol×K | 586.32 | Joback Method |
| cpg | 360.93 | J/mol×K | 621.94 | Joback Method |
| cpg | 373.47 | J/mol×K | 657.55 | Joback Method |
| cpg | 385.26 | J/mol×K | 693.17 | Joback Method |
| cpg | 396.32 | J/mol×K | 728.79 | Joback Method |
| cpg | 406.66 | J/mol×K | 764.40 | Joback Method |
| cpg | 416.30 | J/mol×K | 800.02 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=U307257&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 |
| **McGowan Method:** | http://link.springer.com/article/10.1007/BF02311772 |

# 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 |