# Atomoxetine

**Other names:** Strattera
Benzenepropanamine, N-methyl-«gamma»-(2-methylphenoxy)-, («gamma»R)-
**Inchi:** InChI=1S/C17H21NO/c1-14-8-6-7-11-16(14)19-17(12-13-18-2)15-9-4-3-5-10-15/h3-11,17
**InchiKey:** VHGCDTVCOLNTBX-UHFFFAOYSA-N
**Formula:** C17H21NO
**SMILES:** CNCCC(Oc1ccccc1C)c1ccccc1
**Mol. weight [g/mol]:** 255.35
**CAS:** 83015-26-3

# Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 289.40 | kJ/mol | Joback Method |
| hf | -16.65 | kJ/mol | Joback Method |
| hfus | 30.24 | kJ/mol | Joback Method |
| hvap | 67.11 | kJ/mol | Joback Method |
| log10ws | -4.59 | | Crippen Method |
| logp | 3.725 | | Crippen Method |
| mcvol | 218.720 | ml/mol | McGowan Method |
| pc | 2068.00 | kPa | Joback Method |
| rinpol | 1976.90 | | NIST Webbook |
| rinpol | 1976.90 | | NIST Webbook |
| tb | 718.85 | K | Joback Method |
| tc | 945.12 | K | Joback Method |
| tf | 406.60 | K | Joback Method |
| vc | 0.819 | m3/kmol | Joback Method |

# Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 609.06 | J/mol×K | 718.85 | Joback Method |
| cpg | 626.66 | J/mol×K | 756.56 | Joback Method |
| cpg | 643.00 | J/mol×K | 794.27 | Joback Method |
| cpg | 658.12 | J/mol×K | 831.99 | Joback Method |
| cpg | 672.09 | J/mol×K | 869.70 | Joback Method |

| | | | | |
|---|---|---|---|---|
| cpg | 684.95 | J/mol×K | 907.41 | Joback Method |
| cpg | 696.77 | J/mol×K | 945.12 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C83015263&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

| | |
|---|---|
| **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 |