# Tapentadol

**Other names:** Phenol, 3-[(1R,2R)-3-(dimethylamino)-1-ethyl-2-methylpropyl]-
**Inchi:** InChI=1S/C14H23NO/c1-5-14(11(2)10-15(3)4)12-7-6-8-13(16)9-12/h6-9,11,14,16H,5,10H
**InchiKey:** KWTWDQCKEHXFFR-UHFFFAOYSA-N
**Formula:** C14H23NO
**SMILES:** CCC(c1cccc(O)c1)C(C)CN(C)C
**Mol. weight [g/mol]:** 221.34
**CAS:** 175591-23-8

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 130.69 | kJ/mol | Joback Method |
| hf | -216.10 | kJ/mol | Joback Method |
| hfus | 27.82 | kJ/mol | Joback Method |
| hvap | 63.31 | kJ/mol | Joback Method |
| log10ws | -2.63 | | Crippen Method |
| logp | 3.084 | | Crippen Method |
| mcvol | 200.210 | ml/mol | McGowan Method |
| pc | 2338.29 | kPa | Joback Method |
| rinpol | 1697.20 | | NIST Webbook |
| rinpol | 1697.20 | | NIST Webbook |
| tb | 638.58 | K | Joback Method |
| tc | 848.39 | K | Joback Method |
| tf | 388.15 | K | Joback Method |
| vc | 0.683 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 544.66 | J/mol×K | 638.58 | Joback Method |
| cpg | 562.01 | J/mol×K | 673.55 | Joback Method |
| cpg | 578.30 | J/mol×K | 708.52 | Joback Method |
| cpg | 593.61 | J/mol×K | 743.49 | Joback Method |
| cpg | 608.04 | J/mol×K | 778.45 | Joback Method |
| cpg | 621.66 | J/mol×K | 813.42 | Joback Method |

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|---|---|---|---|---|
| cpg | 634.58 | J/mol×K | 848.39 | 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=C175591238&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |

# 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 |