# N-Desmethyl-cis-tramadol

**Inchi:** InChI=1S/C15H23NO2/c1-16-11-13-6-3-4-9-15(13,17)12-7-5-8-14(10-12)18-2/h5,7-8,10,
**InchiKey:** VUMQHLSPUAFKKK-ZFWWWQNUSA-N
**Formula:** C15H23NO2
**SMILES:** CNCC1CCCCC1(O)c1cccc(OC)c1
**Mol. weight [g/mol]:** 249.35
**CAS:** 75377-45-6

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 37.02 | kJ/mol | Joback Method |
| hf | -309.63 | kJ/mol | Joback Method |
| hfus | 25.24 | kJ/mol | Joback Method |
| hvap | 76.42 | kJ/mol | Joback Method |
| log10ws | -3.18 | | Crippen Method |
| logp | 2.292 | | Crippen Method |
| mcvol | 209.310 | ml/mol | McGowan Method |
| pc | 2410.00 | kPa | Joback Method |
| rinpol | 2024.90 | | NIST Webbook |
| tb | 754.15 | K | Joback Method |
| tc | 969.45 | K | Joback Method |
| tf | 460.50 | K | Joback Method |
| vc | 0.769 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 638.05 | J/mol×K | 754.15 | Joback Method |
| cpg | 655.37 | J/mol×K | 790.03 | Joback Method |
| cpg | 671.91 | J/mol×K | 825.92 | Joback Method |
| cpg | 687.78 | J/mol×K | 861.80 | Joback Method |
| cpg | 703.10 | J/mol×K | 897.68 | Joback Method |
| cpg | 717.98 | J/mol×K | 933.56 | Joback Method |
| cpg | 732.53 | J/mol×K | 969.45 | Joback Method |

# Sources

| | |
|---|---|
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=C75377456&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 |

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