# Norscopolamine

**Inchi:** InChI=1S/C16H19NO4/c18-8-11(9-4-2-1-3-5-9)16(19)20-10-6-12-14-15(21-14)13(7-10)17
**InchiKey:** MOYZEMOPQDTDHA-HZDUJQEKSA-N
**Formula:** C16H19NO4
**SMILES:** O=C(OC1CC2NC(C1)C1OC21)C(CO)c1ccccc1
**Mol. weight [g/mol]:** 289.33

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -8.51 | kJ/mol | Joback Method |
| hf | -455.82 | kJ/mol | Joback Method |
| hfus | 48.70 | kJ/mol | Joback Method |
| hvap | 89.32 | kJ/mol | Joback Method |
| log10ws | -2.23 | | Crippen Method |
| logp | 0.576 | | Crippen Method |
| mcvol | 209.120 | ml/mol | McGowan Method |
| pc | 2665.27 | kPa | Joback Method |
| rinpol | 2246.00 | | NIST Webbook |
| rinpol | 2246.00 | | NIST Webbook |
| tb | 846.57 | K | Joback Method |
| tc | 1069.63 | K | Joback Method |
| tf | 591.42 | K | Joback Method |
| vc | 0.787 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 702.09 | J/mol×K | 846.57 | Joback Method |
| cpg | 716.52 | J/mol×K | 883.75 | Joback Method |
| cpg | 730.04 | J/mol×K | 920.92 | Joback Method |
| cpg | 742.75 | J/mol×K | 958.10 | Joback Method |
| cpg | 754.78 | J/mol×K | 995.28 | Joback Method |
| cpg | 766.22 | J/mol×K | 1032.45 | Joback Method |
| cpg | 777.18 | J/mol×K | 1069.63 | Joback Method |

# Sources

| | |
|---|---|
| **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=R421804&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 |