# O-nitro carbanilic acid, isopulegol ester

**Inchi:** InChI=1S/C17H22N2O4/c1-11(2)13-9-8-12(3)10-16(13)23-17(20)18-14-6-4-5-7-15(14)19
**InchiKey:** MMHUSMJEBKAWJI-UHFFFAOYSA-N
**Formula:** C17H22N2O4
**SMILES:** C=C(C)C1CCC(C)CC1OC(=O)Nc1ccccc1[N+](=O)[O-]
**Mol. weight [g/mol]:** 318.37
**CAS:** 98074-68-1

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | 174.38 | kJ/mol | Joback Method |
| hf | -241.96 | kJ/mol | Joback Method |
| hfus | 44.07 | kJ/mol | Joback Method |
| hvap | 87.78 | kJ/mol | Joback Method |
| log10ws | -5.53 | | Crippen Method |
| logp | 4.524 | | Crippen Method |
| mcvol | 246.310 | ml/mol | McGowan Method |
| pc | 1928.74 | kPa | Joback Method |
| tb | 905.09 | K | Joback Method |
| tc | 1151.40 | K | Joback Method |
| tf | 571.90 | K | Joback Method |
| vc | 0.933 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 803.25 | J/mol×K | 905.09 | Joback Method |
| cpg | 818.08 | J/mol×K | 946.14 | Joback Method |
| cpg | 831.27 | J/mol×K | 987.19 | Joback Method |
| cpg | 842.88 | J/mol×K | 1028.25 | Joback Method |
| cpg | 852.94 | J/mol×K | 1069.30 | Joback Method |
| cpg | 861.53 | J/mol×K | 1110.35 | Joback Method |
| cpg | 868.70 | J/mol×K | 1151.40 | Joback Method |

# Sources

| | |
|---|---|
| **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=C98074681&Units=SI |
| **Crippen Method:** | http://pubs.acs.org/doi/abs/10.1021/ci990307l |
| **Crippen Method:** | https://www.chemeo.com/doc/models/crippen_log10ws |

# 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 |
| **tb:** | Normal Boiling Point Temperature |
| **tc:** | Critical Temperature |
| **tf:** | Normal melting (fusion) point |
| **vc:** | Critical Volume |