# PROPAFENONE-H2O, M(DESAMINO-HO-), AC

**Inchi:** InChI=1S/C20H20O4/c1-16(21)23-14-7-15-24-20-11-6-5-10-18(20)19(22)13-12-17-8-3-2
**InchiKey:** JNJLPJKSKKKSAY-VIZOYTHASA-N
**Formula:** C20H20O4
**SMILES:** CC(=O)OCC=COc1ccccc1C(=O)CCc1ccccc1
**Mol. weight [g/mol]:** 324.37

## Physical Properties

| Property code | Value | Unit | Source |
|---|---|---|---|
| gf | -54.91 | kJ/mol | Joback Method |
| hf | -366.92 | kJ/mol | Joback Method |
| hfus | 41.02 | kJ/mol | Joback Method |
| hvap | 83.60 | kJ/mol | Joback Method |
| log10ws | -5.17 | | Crippen Method |
| logp | 3.958 | | Crippen Method |
| mcvol | 255.720 | ml/mol | McGowan Method |
| pc | 1815.41 | kPa | Joback Method |
| rinpol | 2715.00 | | NIST Webbook |
| rinpol | 2715.00 | | NIST Webbook |
| tb | 872.08 | K | Joback Method |
| tc | 1102.04 | K | Joback Method |
| tf | 519.76 | K | Joback Method |
| vc | 0.968 | m3/kmol | Joback Method |

## Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---|---|---|---|---|
| cpg | 754.10 | J/mol×K | 872.08 | Joback Method |
| cpg | 811.53 | J/mol×K | 1063.71 | Joback Method |
| cpg | 802.24 | J/mol×K | 1025.39 | Joback Method |
| cpg | 791.90 | J/mol×K | 987.06 | Joback Method |
| cpg | 780.48 | J/mol×K | 948.73 | Joback Method |
| cpg | 767.90 | J/mol×K | 910.41 | Joback Method |
| cpg | 819.85 | J/mol×K | 1102.04 | Joback Method |
| dvisc | 0.0000490 | Pa×s | 872.08 | Joback Method |

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|---|---|---|---|---|
| dvisc | 0.0000624 | Pa×s | 813.36 | Joback Method |
| dvisc | 0.0000826 | Pa×s | 754.64 | Joback Method |
| dvisc | 0.0001145 | Pa×s | 695.92 | Joback Method |
| dvisc | 0.0001685 | Pa×s | 637.20 | Joback Method |
| dvisc | 0.0002684 | Pa×s | 578.48 | Joback Method |
| dvisc | 0.0004750 | Pa×s | 519.76 | Joback Method |

# Sources

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|---|---|
| **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 |
| **NIST Webbook:** | http://webbook.nist.gov/cgi/cbook.cgi?ID=R255375&Units=SI |

# Legend

| | |
|---|---|
| **cpg:** | Ideal gas heat capacity |
| **dvisc:** | Dynamic viscosity |
| **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 |