

Norpropoxypheneamide

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| Inchi: | InChI=1S/C20H23NO3/c1-3-19(23)24-20(15-21(2)16-22,18-12-8-5-9-13-18)14-17-10-6-4 |
| InchiKey: | OBVKZRJOBNSRRS-UHFFFAOYSA-N |
| Formula: | C20H23NO3 |
| SMILES: | CCC(=O)OC(Cc1ccccc1)(CN(C)C=O)c1ccccc1 |
| Mol. weight [g/mol]: | 325.40 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|---------|----------------|
| gf | 122.52 | kJ/mol | Joback Method |
| hf | -254.67 | kJ/mol | Joback Method |
| hfus | 36.32 | kJ/mol | Joback Method |
| hvap | 81.29 | kJ/mol | Joback Method |
| log10ws | -3.78 | | Crippen Method |
| logp | 3.166 | | Crippen Method |
| mcvol | 264.130 | ml/mol | McGowan Method |
| pc | 1827.85 | kPa | Joback Method |
| rinpol | 2527.00 | | NIST Webbook |
| rinpol | 2527.00 | | NIST Webbook |
| rinpol | 2505.00 | | NIST Webbook |
| rinpol | 2507.00 | | NIST Webbook |
| tb | 844.52 | K | Joback Method |
| tc | 1072.18 | K | Joback Method |
| tf | 517.05 | K | Joback Method |
| vc | 0.988 | m3/kmol | Joback Method |

Temperature Dependent Properties

| Property code | Value | Unit | Temperature [K] | Source |
|---------------|--------|---------|-----------------|---------------|
| cpg | 797.47 | J/molxK | 844.52 | Joback Method |
| cpg | 812.53 | J/molxK | 882.46 | Joback Method |
| cpg | 826.37 | J/molxK | 920.41 | Joback Method |
| cpg | 839.09 | J/molxK | 958.35 | Joback Method |
| cpg | 850.80 | J/molxK | 996.29 | Joback Method |
| cpg | 861.60 | J/molxK | 1034.23 | 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=U123368&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |

Legend

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|-----------------|---|
| 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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<https://www.chemeo.com/cid/40-561-4/Norpropoxypheneamide.pdf>

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