

# N,N-Dimethyl-N'-(3-nitrophenyl)-benzamidine

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C15H15N3O2/c1-17(2)15(12-7-4-3-5-8-12)16-13-9-6-10-14(11-13)18(19)20/h3 |
| InchiKey:            | IIVMJFUTKMACDI-FOCLMDBBSA-N                                                      |
| Formula:             | C15H15N3O2                                                                       |
| SMILES:              | CN(C)C(=Nc1cccc([N+](=O)[O-])c1)c1ccccc1                                         |
| Mol. weight [g/mol]: | 269.30                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 237.86  | kJ/mol | Joback Method  |
| hvap          | 76.23   | kJ/mol | Joback Method  |
| log10ws       | -3.89   |        | Crippen Method |
| logp          | 3.235   |        | Crippen Method |
| mcvol         | 207.770 | ml/mol | McGowan Method |
| pc            | 2265.42 | kPa    | Joback Method  |
| rinpol        | 2291.00 |        | NIST Webbook   |
| rinpol        | 2291.00 |        | NIST Webbook   |
| tb            | 841.78  | K      | Joback Method  |
| tc            | 1108.62 | K      | Joback Method  |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| McGowan Method: | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=R158779&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R158779&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|       |                                                 |
|-------|-------------------------------------------------|
| hf:   | Enthalpy of formation at standard conditions    |
| hvap: | Enthalpy of vaporization at standard conditions |

|                 |                                     |
|-----------------|-------------------------------------|
| <b>log10ws:</b> | Log10 of Water solubility in mol/l  |
| <b>logp:</b>    | Octanol/Water partition coefficient |
| <b>mcvol:</b>   | McGowan's characteristic volume     |
| <b>pc:</b>      | Critical Pressure                   |
| <b>rinpol:</b>  | Non-polar retention indices         |
| <b>tb:</b>      | Normal Boiling Point Temperature    |
| <b>tc:</b>      | Critical Temperature                |

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