

# N,N-Dimethyl-N'-(3-chlorophenyl)-p-methoxybenz

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C16H17ClN2O/c1-19(2)16(12-7-9-15(20-3)10-8-12)18-14-6-4-5-13(17)11-14/h |
| InchiKey:            | GBSUGWKQSCSKHY-FBMGVBCBSA-N                                                      |
| Formula:             | C16H17ClN2O                                                                      |
| SMILES:              | COc1ccc(C(=Nc2cccc(Cl)c2)N(C)C)cc1                                               |
| Mol. weight [g/mol]: | 288.77                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 68.55   | kJ/mol | Joback Method  |
| hvap          | 69.32   | kJ/mol | Joback Method  |
| log10ws       | -4.04   |        | Crippen Method |
| logp          | 3.989   |        | Crippen Method |
| mcvol         | 222.550 | ml/mol | McGowan Method |
| pc            | 1927.05 | kPa    | Joback Method  |
| rinpol        | 2234.00 |        | NIST Webbook   |
| tb            | 777.65  | K      | Joback Method  |
| tc            | 1021.73 | K      | Joback Method  |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Joback Method:  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |
| 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=R158635&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R158635&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |

## Legend

|          |                                                 |
|----------|-------------------------------------------------|
| hf:      | Enthalpy of formation at standard conditions    |
| hvap:    | Enthalpy of vaporization at standard conditions |
| log10ws: | 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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