

# Propanamide, N-(3-methylphenyl)-3-phenyl-

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Inchi:               | InChI=1S/C16H17NO/c1-13-6-5-9-15(12-13)17-16(18)11-10-14-7-3-2-4-8-14/h2-9,12H,1 |
| InchiKey:            | AZCPQNSZMBNXPE-UHFFFAOYSA-N                                                      |
| Formula:             | C16H17NO                                                                         |
| SMILES:              | <chem>Cc1cccc(N=C(O)CCc2ccccc2)c1</chem>                                         |
| Mol. weight [g/mol]: | 239.31                                                                           |

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 8.22    | kJ/mol | Joback Method  |
| hvap          | 76.50   | kJ/mol | Joback Method  |
| log10ws       | -4.37   |        | Crippen Method |
| logp          | 4.216   |        | Crippen Method |
| mcpvol        | 200.330 | ml/mol | McGowan Method |
| pc            | 2235.52 | kPa    | Joback Method  |
| rinpol        | 2177.00 |        | NIST Webbook   |
| rinpol        | 2177.00 |        | NIST Webbook   |
| tb            | 792.56  | K      | Joback Method  |
| tc            | 1021.66 | K      | Joback Method  |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U308115&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U308115&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>                         |
| 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>                     |

## 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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