

# p-methylbenzylidene-(3-nitrophenyl)-amine

**Inchi:** InChI=1S/C14H12N2O2/c1-11-5-7-12(8-6-11)10-15-13-3-2-4-14(9-13)16(17)18/h2-10H,1  
**InchiKey:** MTKMJIIIUICKAX-UHFFFAOYSA-N  
**Formula:** C14H12N2O2  
**SMILES:** Cc1ccc(C=Nc2cccc([N+](=O)[O-])c2)cc1  
**Mol. weight [g/mol]:** 240.26

## Physical Properties

| Property code | Value   | Unit   | Source         |
|---------------|---------|--------|----------------|
| hf            | 189.29  | kJ/mol | Joback Method  |
| hvap          | 72.54   | kJ/mol | Joback Method  |
| log10ws       | -4.46   |        | Crippen Method |
| logp          | 3.654   |        | Crippen Method |
| mcvol         | 183.700 | ml/mol | McGowan Method |
| pc            | 2443.48 | kPa    | Joback Method  |
| rinpol        | 2348.00 |        | NIST Webbook   |
| tb            | 811.56  | K      | Joback Method  |
| tc            | 1085.88 | K      | Joback Method  |

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>  
**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=R160257&Units=SI>  
**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>  
**Crippen Method:** [https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)  
**Joback Method:** [https://en.wikipedia.org/wiki/Joback\\_method](https://en.wikipedia.org/wiki/Joback_method)

## 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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