

# 2,4,5-Trifluoro-3-methoxybenzamide, N-(4-bromophenyl)-

**Inchi:** InChI=1S/C14H9BrF3NO2/c1-21-13-11(17)9(6-10(16)12(13)18)14(20)19-8-4-2-7(15)3-5-  
**InchiKey:** JIZGNYVSUYKYAF-UHFFFAOYSA-N  
**Formula:** C14H9BrF3NO2  
**SMILES:** COc1c(F)c(F)cc(C(=O)Nc2ccc(Br)cc2)c1F  
**Mol. weight [g/mol]:** 360.13

## Physical Properties

| Property code | Value   | Unit    | Source         |
|---------------|---------|---------|----------------|
| gf            | -470.97 | kJ/mol  | Joback Method  |
| hf            | -669.91 | kJ/mol  | Joback Method  |
| hfus          | 40.56   | kJ/mol  | Joback Method  |
| hvap          | 74.20   | kJ/mol  | Joback Method  |
| log10ws       | -5.73   |         | Crippen Method |
| logp          | 4.127   |         | Crippen Method |
| mcvol         | 200.830 | ml/mol  | McGowan Method |
| pc            | 2545.61 | kPa     | Joback Method  |
| rinpol        | 2420.00 |         | NIST Webbook   |
| tb            | 788.41  | K       | Joback Method  |
| tc            | 1013.08 | K       | Joback Method  |
| tf            | 549.37  | K       | Joback Method  |
| vc            | 0.778   | m3/kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source        |
|---------------|--------|---------|-----------------|---------------|
| cpg           | 516.14 | J/mol×K | 788.41          | Joback Method |
| cpg           | 526.55 | J/mol×K | 825.85          | Joback Method |
| cpg           | 536.10 | J/mol×K | 863.30          | Joback Method |
| cpg           | 544.81 | J/mol×K | 900.74          | Joback Method |
| cpg           | 552.71 | J/mol×K | 938.19          | Joback Method |
| cpg           | 559.82 | J/mol×K | 975.63          | Joback Method |
| cpg           | 566.17 | J/mol×K | 1013.08         | Joback Method |

# Sources

|                        |                                                                                                                                           |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| <b>McGowan Method:</b> | <a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>                     |
| <b>NIST Webbook:</b>   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U358071&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U358071&amp;Units=SI</a> |
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| <b>Crippen Method:</b> | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| <b>Joback Method:</b>  | <a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>                                     |

## Legend

|                 |                                                 |
|-----------------|-------------------------------------------------|
| <b>cpg:</b>     | Ideal gas heat capacity                         |
| <b>gf:</b>      | Standard Gibbs free energy of formation         |
| <b>hf:</b>      | Enthalpy of formation at standard conditions    |
| <b>hfus:</b>    | Enthalpy of fusion at standard conditions       |
| <b>hvap:</b>    | 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                            |
| <b>tf:</b>      | Normal melting (fusion) point                   |
| <b>vc:</b>      | Critical Volume                                 |

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