

# 4-Butyl-N-(4-ethoxybenzylidene)aniline

|                      |                                                                                                                                                                                                                                                                                                                                                                   |
|----------------------|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | p-Ethoxybenzylidene p-butylaniline<br>Benzenamine, 4-butyl-N-[(4-ethoxyphenyl)methylene]-<br>4-Butyl-N-[(4-ethoxyphenyl)methylidene]aniline<br>N-p-Ethoxybenzylidene-p-butylaniline<br>N-(4'-Ethoxybenzylidene)-4-n-butylaniline<br>N-(4-Ethoxybenzylidene)-4-butylaniline<br>p-[(p-Ethoxybenzylidene)amino]butylbenzene<br>N-p-Ethoxybenzylidene-p'-butylaniline |
| Inchi:               | InChI=1S/C19H23NO/c1-3-5-6-16-7-11-18(12-8-16)20-15-17-9-13-19(14-10-17)21-4-2/h                                                                                                                                                                                                                                                                                  |
| InchiKey:            | DBOAVDSSZWGDGTH-UHFFFAOYSA-N                                                                                                                                                                                                                                                                                                                                      |
| Formula:             | C19H23NO                                                                                                                                                                                                                                                                                                                                                          |
| SMILES:              | CCCCc1ccc(N=Cc2ccc(OCC)cc2)cc1                                                                                                                                                                                                                                                                                                                                    |
| Mol. weight [g/mol]: | 281.39                                                                                                                                                                                                                                                                                                                                                            |
| CAS:                 | 29743-08-6                                                                                                                                                                                                                                                                                                                                                        |

## Physical Properties

| Property code | Value         | Unit    | Source         |
|---------------|---------------|---------|----------------|
| hf            | -35.37        | kJ/mol  | Joback Method  |
| hvap          | 69.49         | kJ/mol  | Joback Method  |
| log10ws       | -5.52         |         | Crippen Method |
| logp          | 5.178         |         | Crippen Method |
| mcvol         | 242.600       | ml/mol  | McGowan Method |
| pc            | 1559.81       | kPa     | Joback Method  |
| ss            | 421.79        | J/mol×K | NIST Webbook   |
| tb            | 796.54        | K       | Joback Method  |
| tc            | 1025.77       | K       | Joback Method  |
| tt            | 305.62 ± 0.02 | K       | NIST Webbook   |

## Temperature Dependent Properties

| Property code | Value  | Unit    | Temperature [K] | Source       |
|---------------|--------|---------|-----------------|--------------|
| cps           | 429.09 | J/mol×K | 298.15          | NIST Webbook |
| cps           | 425.00 | J/mol×K | 300.00          | NIST Webbook |
| hfust         | 27.09  | kJ/mol  | 305.62          | NIST Webbook |

|       |       |         |        |              |
|-------|-------|---------|--------|--------------|
| hfust | 27.09 | kJ/mol  | 305.62 | NIST Webbook |
| sfust | 88.71 | J/mol×K | 305.62 | NIST Webbook |
| sfust | 88.71 | J/mol×K | 305.62 | NIST Webbook |

## Sources

|                        |                                                                                                                                               |
|------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                     |
| <b>Crippen Method:</b> | <a href="https://www.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>                                         |
| <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=C29743086&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C29743086&amp;Units=SI</a> |

## Legend

|                 |                                                  |
|-----------------|--------------------------------------------------|
| <b>cps:</b>     | Solid phase heat capacity                        |
| <b>hf:</b>      | Enthalpy of formation at standard conditions     |
| <b>hfust:</b>   | Enthalpy of fusion at a given temperature        |
| <b>hvac:</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>sfust:</b>   | Entropy of fusion at a given temperature         |
| <b>ss:</b>      | Solid phase molar entropy at standard conditions |
| <b>tb:</b>      | Normal Boiling Point Temperature                 |
| <b>tc:</b>      | Critical Temperature                             |
| <b>tt:</b>      | Triple Point Temperature                         |

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