

# Benzoic acid, 3-di(3-methylbutyl)amino-, 3-methylbutyl ester

|                             |  |
|-----------------------------|--|
| <b>Inchi:</b>               | InChI=1S/C22H37NO2/c1-17(2)10-13-23(14-11-18(3)4)21-9-7-8-20(16-21)22(24)25-15-1 |
| <b>InchiKey:</b>            | JUEMSBZDBDVFDFU-UHFFFAOYSA-N   |
| <b>Formula:</b>             | C22H37NO2  |
| <b>SMILES:</b>              | CC(C)CCOC(=O)c1cccc(N(CCC(C)C)CCC(C)C)c1   |
| <b>Mol. weight [g/mol]:</b> | 347.53   |

## Physical Properties

| Property code | Value   | Unit                 | Source         |
|---------------|---------|----------------------|----------------|
| gf            | 106.68  | kJ/mol               | Joback Method  |
| hf            | -465.46 | kJ/mol               | Joback Method  |
| hfus          | 41.63   | kJ/mol               | Joback Method  |
| hvap          | 77.54   | kJ/mol               | Joback Method  |
| log10ws       | -5.92   |                      | Crippen Method |
| logp          | 5.788   |                      | Crippen Method |
| mvol          | 314.500 | ml/mol               | McGowan Method |
| pc            | 1152.22 | kPa                  | Joback Method  |
| rmpol         | 2375.00 |                      | NIST Webbook   |
| rmpol         | 2375.00 |                      | NIST Webbook   |
| tb            | 821.83  | K                    | Joback Method  |
| tc            | 1019.18 | K                    | Joback Method  |
| tf            | 436.27  | K                    | Joback Method  |
| vc            | 1.183   | m <sup>3</sup> /kmol | Joback Method  |

## Temperature Dependent Properties

| Property code | Value   | Unit    | Temperature [K] | Source        |
|---------------|---------|---------|-----------------|---------------|
| cpg           | 989.88  | J/molxK | 821.83          | Joback Method |
| cpg           | 1009.04 | J/molxK | 854.72          | Joback Method |
| cpg           | 1027.01 | J/molxK | 887.61          | Joback Method |
| cpg           | 1043.81 | J/molxK | 920.51          | Joback Method |
| cpg           | 1059.50 | J/molxK | 953.40          | Joback Method |
| cpg           | 1074.13 | J/molxK | 986.29          | Joback Method |
| cpg           | 1087.75 | J/molxK | 1019.18         | Joback Method |

# Sources

|                        |   |
|------------------------|---|
| <b>Crippen Method:</b> | <a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=U375449&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U375449&amp;Units=SI</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>hvp:</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>rinp:</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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