

# Benzoic acid, 3-amino-, tert-butyldimethylsilyl ester

|                      |  |
|----------------------|--|
| Inchi:               | InChI=1S/C13H21NO2Si/c1-13(2,3)17(4,5)16-12(15)10-7-6-8-11(14)9-10/h6-9H,14H2,1- |
| InchiKey:            | LEMFTLBDBKRTJX-UHFFFAOYSA-N  |
| Formula:             | C13H21NO2Si  |
| SMILES:              | CC(C)(C)[Si](C)(C)OC(=O)c1cccc(N)c1  |
| Mol. weight [g/mol]: | 251.40   |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.49   |      | Crippen Method |
| logp          | 3.431   |      | Crippen Method |
| rinpol        | 1844.00 |      | NIST Webbook   |
| rinpol        | 1844.00 |      | NIST Webbook   |

## Sources

|                 |   |
|-----------------|---|
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                         |
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U374524&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U374524&amp;Units=SI</a> |
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</a>                                 |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |
| rinpol:  | Non-polar retention indices         |

Latest version available from:

<https://www.chemeo.com/cid/114-612-5/Benzoic-acid-3-amino-tert-butyldimethylsilyl-ester.pdf>

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