

# tert-Butyldimethylsilyl 4-nitrobenzoate

|                      |                                                                                  |
|----------------------|----------------------------------------------------------------------------------|
| Other names:         | 4-Nitrobenzoic acid, tert-butyldimethylsilyl ester                               |
| Inchi:               | InChI=1S/C13H19NO4Si/c1-13(2,3)19(4,5)18-12(15)10-6-8-11(9-7-10)14(16)17/h6-9H,1 |
| InchiKey:            | TVYJISKNYVTYMG-UHFFFAOYSA-N                                                      |
| Formula:             | C13H19NO4Si                                                                      |
| SMILES:              | CC(C)(C)[Si](C)(C)OC(=O)c1ccc([N+](=O)[O-])cc1                                   |
| Mol. weight [g/mol]: | 281.38                                                                           |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -2.51   |      | Crippen Method |
| logp          | 3.757   |      | Crippen Method |
| rinpol        | 1866.00 |      | NIST Webbook   |
| rinpol        | 1866.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                           |
|-----------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | <a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</a>                                 |
| 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=U373050&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373050&amp;Units=SI</a> |

## Legend

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

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