

# 3,4-Dimethylbenzoic acid, trimethylsilyl ester

|                      |                                                                        |
|----------------------|------------------------------------------------------------------------|
| Other names:         | 3,4-Dimethylbenzoic acid, TMS                                          |
| Inchi:               | InChI=1S/C12H18O2Si/c1-9-6-7-11(8-10(9)2)12(13)14-15(3,4)5/h6-8H,1-5H3 |
| InchiKey:            | GVQLTVPJABMNKV-UHFFFAOYSA-N                                            |
| Formula:             | C12H18O2Si                                                             |
| SMILES:              | <chem>Cc1ccc(C(=O)O[Si](C)(C)C)cc1C</chem>                             |
| Mol. weight [g/mol]: | 222.36                                                                 |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -1.55   |      | Crippen Method |
| logp          | 3.295   |      | Crippen Method |
| rinpol        | 1493.00 |      | NIST Webbook   |
| rinpol        | 1493.00 |      | 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=U373013&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U373013&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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