

# Benzenepropanoic acid, trimethylsilyl ester

|                      |                                                                                                                                                                                                     |
|----------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| Other names:         | Hydrocinnamic acid, trimethylsilyl ester<br>Trimethylsilyl 3-phenylpropanoate<br>Dihydrocinnamic acid, TMS<br>Dihydrocinnamic (benzenepropanoic) acid, TMS<br>Benzenepropanoic acid, tms derivative |
| Inchi:               | InChI=1S/C12H18O2Si/c1-15(2,3)14-12(13)10-9-11-7-5-4-6-8-11/h4-8H,9-10H2,1-3H3                                                                                                                      |
| InchiKey:            | GRONVOGSDOJOMG-UHFFFAOYSA-N                                                                                                                                                                         |
| Formula:             | C12H18O2Si                                                                                                                                                                                          |
| SMILES:              | C[Si](C)(C)OC(=O)CCc1ccccc1                                                                                                                                                                         |
| Mol. weight [g/mol]: | 222.36                                                                                                                                                                                              |
| CAS:                 | 21273-15-4                                                                                                                                                                                          |

## Physical Properties

| Property code | Value   | Unit | Source         |
|---------------|---------|------|----------------|
| log10ws       | -0.86   |      | Crippen Method |
| logp          | 2.997   |      | Crippen Method |
| rinpol        | 1414.00 |      | NIST Webbook   |
| rinpol        | 1397.00 |      | NIST Webbook   |
| rinpol        | 1397.00 |      | NIST Webbook   |
| rinpol        | 1414.00 |      | NIST Webbook   |

## Sources

|                 |                                                                                                                                               |
|-----------------|-----------------------------------------------------------------------------------------------------------------------------------------------|
| NIST Webbook:   | <a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C21273154&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C21273154&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>                                     |
| Crippen Method: | <a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>                             |

## Legend

|          |                                     |
|----------|-------------------------------------|
| log10ws: | Log10 of Water solubility in mol/l  |
| logp:    | Octanol/Water partition coefficient |

**rinpol:** Non-polar retention indices

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