

Hydrocinnamic acid, p-(trimethylsiloxy)-, trimethylsilyl ester

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| Other names: | Trimethylsilyl 3-(4-[(trimethylsilyl)oxy]phenyl)propanoate 3-(4-Hydroxyphenyl)propionic acid, (2TMS) 3-(4-Hydroxyphenyl)propionic acid, trimethylsilyl ether, trimethylsilyl ester 4-Hydroxyhydrocinnamic acid, bis-TMS 4-Hydroxyphenylpropionic acid, di-TMS Benzenepropanoic acid, 4-hydroxy, bis-TMS Benzenepropanoic acid, 4-hydroxy, (2TMS) Propanoic acid, 3-(4-hydroxyphenyl), bis-TMS 3-(4-Hydroxyphenyl)propionic acid, TMS Benzenepropanoic acid, 4-trimethylsilyloxy, trimethylsilyl ester Benzenepropanoic acid, 4-hydroxy, TMS 4-Hydroxyhydrocinnamic acid, TMS 4-Hydroxyphenylpropionic acid, TMS Phloretic acid, 2tms derivative |
| Inchi: | InChI=1S/C15H26O3Si2/c1-19(2,3)17-14-10-7-13(8-11-14)9-12-15(16)18-20(4,5)6/h7-8, |
| InchiKey: | NTWRBVRZYOLGDK-UHFFFAOYSA-N |
| Formula: | C15H26O3Si2 |
| SMILES: | C[Si](C)(C)OC(=O)CCc1ccc(O[Si](C)(C)C)cc1 |
| Mol. weight [g/mol]: | 310.54 |
| CAS: | 27750-62-5 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | 0.13 | | Crippen Method |
| logp | 4.211 | | Crippen Method |
| rinpol | 1752.00 | | NIST Webbook |
| rinpol | 1763.00 | | NIST Webbook |
| rinpol | 1750.00 | | NIST Webbook |
| rinpol | 1755.00 | | NIST Webbook |
| rinpol | 1750.10 | | NIST Webbook |
| rinpol | 1762.00 | | NIST Webbook |
| rinpol | 1754.00 | | NIST Webbook |
| rinpol | 1752.00 | | NIST Webbook |
| rinpol | 1762.00 | | NIST Webbook |

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750625&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307I>

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/35-057-0/Hydrocinnamic-acid-p-trimethylsiloxy-trimethylsilyl-ester.pdf>

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