

Trimethylsilyl 3-methylbenzoate

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|-----------------------------|--------------------------------------------------------------------------------------|
| Other names: | Benzoic acid, 3-methyl-, trimethylsilyl ester m-Toluic acid, trimethylsilyl ester |
| Inchi: | InChI=1S/C11H16O2Si/c1-9-6-5-7-10(8-9)11(12)13-14(2,3)4/h5-8H,1-4H3 |
| InchiKey: | MFPKMKJUNGWICD-UHFFFAOYSA-N |
| Formula: | C11H16O2Si |
| SMILES: | Cc1cccc(C(=O)O[Si](C)(C)C)c1 |
| Mol. weight [g/mol]: | 208.33 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.08 | | Crippen Method |
| logp | 2.987 | | Crippen Method |
| rinpol | 1354.00 | | NIST Webbook |

Sources

| | |
|------------------------|-------------------------------------------------------------------------------------------------------------------------------------------|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373033&Units=SI |

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/13-076-3/Trimethylsilyl-3-methylbenzoate.pdf>

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