

But-3-enyl tert-butyldimethylsilyl phthalate

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|-----------------------------|--|
| Other names: | 1,2-Benzenedicarboxylic acid, but-3-enyl tert-butyldimethylsilyl ester |
| Inchi: | InChI=1S/C18H26O4Si/c1-7-8-13-21-16(19)14-11-9-10-12-15(14)17(20)22-23(5,6)18(2,3) |
| InchiKey: | XFVDYWSJIXCFEA-UHFFFAOYSA-N |
| Formula: | C18H26O4Si |
| SMILES: | <chem>C=CCCOC(=O)c1ccccc1C(=O)O[Si](C)(C)C(C)(C)C</chem> |
| Mol. weight [g/mol]: | 334.48 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.21 | | Crippen Method |
| logp | 4.582 | | Crippen Method |
| rinpol | 2044.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373503&Units=SI |
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci9903071 |

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/55-188-3/But-3-enyl-tert-butyldimethylsilyl-phthalate.pdf>

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