

Heptyl trimethylsilyl phthalate

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|-----------------------------|--|
| Other names: | 1,2-Benzenedicarboxylic acid, heptyl trimethylsilyl ester |
| Inchi: | InChI=1S/C18H28O4Si/c1-5-6-7-8-11-14-21-17(19)15-12-9-10-13-16(15)18(20)22-23(2,3) |
| InchiKey: | HEZSKXOBFJKII-UHFFFAOYSA-N |
| Formula: | C18H28O4Si |
| SMILES: | CCCCCCCOC(=O)c1cccc1C(=O)O[Si](C)(C)C |
| Mol. weight [g/mol]: | 336.50 |

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -3.36 | | Crippen Method |
| logp | 4.805 | | Crippen Method |
| rinpol | 2124.00 | | NIST Webbook |

Sources

| | |
|------------------------|---|
| Crippen Method: | http://pubs.acs.org/doi/abs/10.1021/ci990307I |
| Crippen Method: | https://www.chemeo.com/doc/models/crippen_log10ws |
| NIST Webbook: | http://webbook.nist.gov/cgi/cbook.cgi?ID=U373664&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/63-442-1/Heptyl-trimethylsilyl-phthalate.pdf>

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