

(Trimethylsilyl)methyl octanoate

Inchi: InChI=1S/C12H26O2Si/c1-5-6-7-8-9-10-12(13)14-11-15(2,3)4/h5-11H2,1-4H3
InchiKey: JZMNFGBGXTFKDHS-UHFFFAOYSA-N
Formula: C12H26O2Si
SMILES: CCCCCCCC(=O)OC[Si](C)(C)C
Mol. weight [g/mol]: 230.42

Physical Properties

| Property code | Value | Unit | Source |
|---------------|---------|------|----------------|
| log10ws | -1.26 | | Crippen Method |
| logp | 3.767 | | Crippen Method |
| rinpol | 1406.40 | | NIST Webbook |
| rinpol | 1406.40 | | NIST Webbook |

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U333728&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/66-785-8/Trimethylsilyl-methyl-octanoate.pdf>

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