

Pentanoic acid, 5-phenyl, TBDMS

Inchi: InChI=1S/C17H28O2Si/c1-17(2,3)20(4,5)19-16(18)14-10-9-13-15-11-7-6-8-12-15/h6-8,1
InchiKey: MERROXWMQCUWEO-UHFFFAOYSA-N
Formula: C17H28O2Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)CCCCc1ccccc1
Mol. weight [g/mol]: 292.49

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Crippen Method
logp	4.948		Crippen Method
rinpol	1870.00		NIST Webbook
rinpol	1871.00		NIST Webbook
rinpol	1836.00		NIST Webbook
rinpol	1870.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R48560&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/34-853-7/Pentanoic-acid-5-phenyl-TBDMS.pdf>

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