

Prosta-8(12),13-dien-1-oic acid, 9-oxo-15-[(trimethylsilyl)oxy]-, trimethylsilyl ester, (13E,15S)-

Other names: PCB-TMS

InChI: InChI=1S/C26H48O4Si2/c1-8-9-12-15-23(29-31(2,3)4)20-18-22-19-21-25(27)24(22)16-1

InchiKey: IUFSUDSDJVIXHR-KBDAKURLSA-N

Formula: C26H48O4Si2

SMILES: CCCCCC(C=CC1=C(CCCCCC(=O)O[Si](C)(C)C)C(=O)CC1)O[Si](C)(C)C

Mol. weight [g/mol]: 480.83

CAS: 56009-41-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.75		Crippen Method
logp	7.721		Crippen Method
rinpola	2880.00		NIST Webbook
rinpola	2880.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C56009417&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpola: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/123-195-9/Prosta-8-12-13-dien-1-oic-acid-9-oxo-15-trimethylsilyl-oxy-trimethylsilyl-ester>

Generated by Cheméo on 2024-04-30 04:11:41.976938004 +0000 UTC m=+16739550.897515317.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.