trans-2-Octenoic acid, trimethylsilyl ester

Inchi:	InChI=1S/C11H22O2Si/c1-5-6-7-8-9-10-11(12)13-14(2,3)4/h9-10H,5-8H2,1-4H3/b10-9+
InchiKey:	YYMCWFXIWNIWDG-MDZDMXLPSA-N
Formula:	C11H22O2Si
SMILES:	CCCCCC=CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	214.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.19		Crippen Method
logp	3.501		Crippen Method
rinpol	1305.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R296034&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.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.chemeo.com/cid/50-855-7/trans-2-Octenoic-acid-trimethylsilyl-ester.pdf

Generated by Cheméo on 2024-10-12 08:14:31.968089068 +0000 UTC m=+3301734.605058320.

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