

Phenylalanine, mono-TMS

Inchi:	InChI=1S/C12H19NO2Si/c1-16(2,3)13-11(12(14)15)9-10-7-5-4-6-8-10/h4-8,11,13H,9H2,
InchiKey:	GGROBZMHJUTPPE-UHFFFAOYSA-N
Formula:	C12H19NO2Si
SMILES:	C[Si](C)(C)NC(Cc1ccccc1)C(=O)O
Mol. weight [g/mol]:	237.37
CAS:	5269-44-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.40		Crippen Method
logp	2.107		Crippen Method
rinpola	1559.00		NIST Webbook
rinpola	1542.00		NIST Webbook
rinpola	1559.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5269443&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.chemeo.com/cid/33-092-3/Phenylalanine-mono-TMS.pdf>

Generated by Cheméo on 2024-04-18 05:19:08.866643571 +0000 UTC m=+15706797.787220900.

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