

Alanine, phenyl-, trimethylsilyl ester, dl-

Other names:	DL-Phenylalanine, trimethylsilyl ester DI-phenylalanine, tms derivative
Inchi:	InChI=1S/C12H19NO2Si/c1-16(2,3)15-12(14)11(13)9-10-7-5-4-6-8-10/h4-8,11H,9,13H2,
InchiKey:	NBXFAHHUVWSAFQ-UHFFFAOYSA-N
Formula:	C12H19NO2Si
SMILES:	C[Si](C)(C)OC(=O)C(N)Cc1ccccc1
Mol. weight [g/mol]:	237.37
CAS:	2899-42-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.41		Crippen Method
logp	1.935		Crippen Method
rinpol	1559.00		NIST Webbook
rinpol	1554.40		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1563.00		NIST Webbook
rinpol	1559.00		NIST Webbook
rinpol	1554.40		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=C2899425&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.cheméo.com/cid/123-959-1/Alanine-phenyl-trimethylsilyl-ester-dl.pdf>

Generated by Cheméo on 2024-04-27 16:06:05.947064694 +0000 UTC m=+16523214.867642015.

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