

N,O-Bis-(trimethylsilyl)phenylalanine

Other names:	DL-Phenylalanine, N-(trimethylsilyl)-, trimethylsilyl ester Phe, bis-TMS Phenylalanine, di-TMS Phenylalanine (N,O-TMS) Phenylalanine, bis-TMS Phe, TMS Phenylalanine, TMS Phenylalanine, 2tms derivative
Inchi:	InChI=1S/C15H27NO2Si2/c1-19(2,3)16-14(15(17)18-20(4,5)6)12-13-10-8-7-9-11-13/h7-1
InchiKey:	DWNFNBPPSFIIBG-UHFFFAOYSA-N
Formula:	C15H27NO2Si2
SMILES:	C[Si](C)(C)NC(Cc1ccccc1)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	309.55
CAS:	2899-52-7

Physical Properties

Property code	Value	Unit	Source
log10ws	0.53		Crippen Method
logp	3.400		Crippen Method
rinpol	1632.00		NIST Webbook
rinpol	1624.42		NIST Webbook
rinpol	1640.06		NIST Webbook
rinpol	1622.30		NIST Webbook
rinpol	1649.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1625.00		NIST Webbook
rinpol	1621.50		NIST Webbook
rinpol	1635.10		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1636.00		NIST Webbook
rinpol	1640.00		NIST Webbook
rinpol	1621.50		NIST Webbook
rinpol	1624.42		NIST Webbook
rinpol	1624.82		NIST Webbook
rinpol	1622.47		NIST Webbook
ripol	1863.83		NIST Webbook

ripol	1863.65	NIST Webbook
ripol	1863.65	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=C2899527&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpola:	Non-polar retention indices
ripola:	Polar retention indices

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