

2-Pyrrolidone-5-carboxylic acid, trimethylsilyl ester

Other names:	Pyroglutamic acid, tms derivative
Inchi:	InChI=1S/C8H15NO3Si/c1-13(2,3)12-8(11)6-4-5-7(10)9-6/h6H,4-5H2,1-3H3,(H,9,10)
InchiKey:	HYNVOYNMQLZSIW-UHFFFAOYSA-N
Formula:	C8H15NO3Si
SMILES:	C[Si](C)(C)OC(=O)C1CCC(=O)N1
Mol. weight [g/mol]:	201.30

Physical Properties

Property code	Value	Unit	Source
log10ws	0.94		Crippen Method
logp	0.643		Crippen Method
rinpol	1511.00		NIST Webbook
rinpol	1511.00		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=U333171&Units=SI

Legend

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

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