

Glycine, N-(1-oxo-2-butenyl)-, trimethylsilyl ester

Other names:	N-Crotonylglycine, trimethylsilyl ester Trimethylsilyl (2-butenoylamino)acetate Glycine, N-crotonyl, mono-TMS Glycine, N-(1-oxo-2-buten-1-yl)-, trimethylsilyl ester N-crotonylglycine, tms derivative
Inchi:	InChI=1S/C9H17NO3Si/c1-5-6-8(11)10-7-9(12)13-14(2,3)4/h5-6H,7H2,1-4H3,(H,10,11)/b
InchiKey:	YHRQPMFBFLVLRD-AATRIKPKSA-N
Formula:	C9H17NO3Si
SMILES:	CC=CC(=O)NCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	215.32
CAS:	55836-39-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.68		Crippen Method
logp	1.057		Crippen Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		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=C55836390&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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