N-CROTONYLGLYCINE, 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: C/C=C/C(=O)NCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 215.33

Physical Properties

Property code	Value	Unit	Source
logp	1.057		Crippen Method
rinpol	1482.00		NIST Webbook
rinpol	1482.00		NIST Webbook

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55836390&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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