

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

Latest version available from:

<https://www.cheméo.com/cid/22-568-7/N-CROTONYLGLYCINE-TRIMETHYLSILYL-ESTER.pdf>

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