



>>Entry Name: *N,N'*-Bis(*tert*-butoxycarbonyl)guanidine

Synonym(s): Bis(1,1-dimethylethyl) carbonimidoylbiscarbamate, 9CI

CAS Registry Number: 154476-57-0

$[(\text{H}_3\text{C})_3\text{CCOONH}]_2\text{C}=\text{NH}$

Molecular Formula: $\text{C}_{11}\text{H}_{21}\text{N}_3\text{O}_4$

Molecular Weight: 259.305

Accurate Mass: 259.153207

Percentage Composition: C 50.95%; H 8.16%; N 16.20%; O 24.68%

Physical Description: Cryst.

Melting Point: Mp 144°

>>Derivative: *N''*-Trifluoromethanesulfonyl

CAS Registry Number: 207857-15-6

Molecular Formula: $\text{C}_{12}\text{H}_{20}\text{F}_3\text{N}_3\text{O}_6\text{S}$

Molecular Weight: 391.368

Accurate Mass: 391.102491

Percentage Composition: C 36.83%; H 5.15%; F 14.56%; N 10.74%; O 24.53%; S 8.19%

Use/Importance: Reagent for guanidinylation of amines

Melting Point: Mp 114-115°. Mp 124°

>>Derivative: *N''*-Benzyl

CAS Registry Number: 145013-06-5

Molecular Formula: $\text{C}_{18}\text{H}_{27}\text{N}_3\text{O}_4$

Molecular Weight: 349.429

Accurate Mass: 349.200157

Percentage Composition: C 61.87%; H 7.79%; N 12.03%; O 18.31%

Physical Description: Cryst.

Melting Point: Mp 126-127°

References:

Dodd, D.S. *et al.*, *Tet. Lett.*, 1994, **35**, 977-980, (*synth*)

Yong, Y.F. *et al.*, *J.O.C.*, 1997, **62**, 1540-1542, (*benzyl, synth, pmr, cmr*)

Feichtinger, K. *et al.*, *J.O.C.*, 1998, **63**, 8432-8439, (*N''-triflyl, synth, use*)

Org. Synth., 2000, **78**, 91-98, (*N''-triflyl, synth, use*)