Butanoic acid, 4-[bis(trimethylsilyl)amino]-, trimethylsilyl ester

Other names: N,N,O-Tris-(trimethylsilyl)-4-aminobutyric acid
«gamma»-Aminobutyric acid, tri-TMS
Butanoic acid, 4-amino, O,N,N-tris-TMS
GABA 3TMS
Trimethylsilyl 4-(bis(trimethylsilyl)amino)butanoate
4-Aminobutanoic acid, 3tms derivative

Inchi: InChI=1S/C13H33NO2Si3/c1-17(2,3)14(18(4,5)6)12-10-11-13(15)16-19(7,8)9/h10-12H2,

InchiKey: HMZQEGNJWXKANK-UHFFFAOYSA-N

Formula: C13H33NO2Si3

SMILES: C[Si](C)(C)OC(=O)CCCN([Si](C)(C)C)[Si](C)(C)C

Mol. weight [g/mol]: 319.66

CAS: 39508-23-1

Physical Properties

Property code	Value	Unit	Source
log10ws	3.15		Crippen Method
logp	4.117		Crippen Method
rinpol	1541.00		NIST Webbook
rinpol	1542.00		NIST Webbook
rinpol	1542.00		NIST Webbook

Sources

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C39508231&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices