

«gamma»-Aminobutyric acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C13H27NO4Si/c1-7-17-12(16)14-10-8-9-11(15)18-19(5,6)13(2,3)4/h7-10H2,1-
InchiKey: MHGZKVKZOWZLKJ-UHFFFAOYSA-N
Formula: C13H27NO4Si
SMILES: CCOC(=O)NCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 289.44

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.21		Crippen Method
logp	3.061		Crippen Method
rinpol	1779.00		NIST Webbook
rinpol	1779.00		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R562806&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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<https://www.chemeo.com/cid/45-398-1/gamma-Aminobutyric-acid-ethoxycarbonylated-TBDMS.pdf>

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