

Hexanoic acid, 6-[bis(trimethylsilyl)amino]-, trimethylsilyl ester

Other names:	Trimethylsilyl 6-[bis(trimethylsilyl)amino]hexanoate Hexanoic acid, 6-amino, O,N,N-tris-TMS Silanol, trimethyl-, 6-[bis(trimethylsilyl)amino]hexanoate Caproic acid, 6-amino, 3TMS Aminocaproic acid, 3tms derivative
Inchi:	InChI=1S/C15H37NO2Si3/c1-19(2,3)16(20(4,5)6)14-12-10-11-13-15(17)18-21(7,8)9/h10
InchiKey:	CTVFIGVGDCRENC-UHFFFAOYSA-N
Formula:	C15H37NO2Si3
SMILES:	<chem>C[Si](C)(C)OC(=O)CCCCN([Si](C)(C)C)[Si](C)(C)C</chem>
Mol. weight [g/mol]:	347.72
CAS:	25688-76-0

Physical Properties

Property code	Value	Unit	Source
log10ws	2.31		Crippen Method
logp	4.897		Crippen Method
rinpol	1725.00		NIST Webbook
rinpol	1726.00		NIST Webbook
rinpol	1725.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25688760&Units=SI

Legend

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

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