

Terbutaline, tris(trimethylsilyl)ether

Other names:	Terbutaline tris-O-TMS Terbutaline, tris-TMS Terbutaline, 3tms derivative
Inchi:	InChI=1S/C21H43NO3Si3/c1-21(2,3)22-16-20(25-28(10,11)12)17-13-18(23-26(4,5)6)15-
InchiKey:	HCOIHNBLVDOGQK-UHFFFAOYSA-N
Formula:	C21H43NO3Si3
SMILES:	CC(C)(C)NCC(O[Si](C)(C)C)c1cc(O[Si](C)(C)C)cc(O[Si](C)(C)C)c1
Mol. weight [g/mol]:	441.83
CAS:	125319-35-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.12		Crippen Method
logp	6.395		Crippen Method

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C125319359&Units=SI

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient

Latest version available from:

<https://www.cheméo.com/cid/80-205-5/Terbutaline-tris-trimethylsilyl-ether.pdf>

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