

dl-Metanephrine, bis(trimethylsilyl) ether

Other names:	Metanephrine, 2tms derivative
Inchi:	InChI=1S/C16H31NO3Si2/c1-17-12-16(20-22(6,7)8)13-9-10-14(15(11-13)18-2)19-21(3,4
InchiKey:	AXSFPBKFSQWQKQ-UHFFFAOYSA-N
Formula:	C16H31NO3Si2
SMILES:	CNCC(O[Si](C)(C)C)c1ccc(O[Si](C)(C)C)c(OC)c1
Mol. weight [g/mol]:	341.59

Physical Properties

Property code	Value	Unit	Source
log10ws	0.14		Crippen Method
logp	4.021		Crippen Method
rinpol	1787.60		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U334022&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

Latest version available from:

<https://www.chemeo.com/cid/11-298-9/dl-Metanephrine-bis-trimethylsilyl-ether.pdf>

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