

dl-Metanephrine, bis(tert-butyldimethylsilyl) ether

Other names:	Metanephrine, 2tbdms derivative
Inchi:	InChI=1S/C22H43NO3Si2/c1-21(2,3)27(9,10)25-18-14-13-17(15-19(18)24-8)20(16-23-7)
InchiKey:	ZLTAOLBLYQYGNN-UHFFFAOYSA-N
Formula:	C22H43NO3Si2
SMILES:	CNCC(O[Si](C)(C)C(C)(C)C)c1ccc(O[Si](C)(C)C(C)(C)C)c(OC)c1
Mol. weight [g/mol]:	425.75

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.37		Crippen Method
logp	6.361		Crippen Method
rinpol	2239.80		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U334024&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/18-353-0/dl-Metanephrine-bis-tert-butyldimethylsilyl-ether.pdf>

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