

Clenbuterol, tert-butyl dimethylsilyl ether

Other names:	Clenbuterol, tbdms derivative
Inchi:	InChI=1S/C18H32Cl2N2OSi/c1-17(2,3)22-11-15(23-24(7,8)18(4,5)6)12-9-13(19)16(21)14
InchiKey:	JBSYMPUCORTAKN-UHFFFAOYSA-N
Formula:	C18H32Cl2N2OSi
SMILES:	CC(C)(C)NCC(O[Si](C)(C)C(C)(C)C)c1cc(Cl)c(N)c(Cl)c1
Mol. weight [g/mol]:	391.45

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.36		Crippen Method
logp	6.027		Crippen Method
rinsol	2208.20		NIST Webbook
rinsol	2208.20		NIST Webbook

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=U333972&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/30-213-1/Clenbuterol-tert-butyl dimethylsilyl-ether.pdf>

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