Clenbuterol, tert-butyldimethylsilyl 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
rinpol	2208.20		NIST Webbook
rinpol	2208.20		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.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
rinpol: Non-polar retention indices