

Clenbuterol TMS derivative

Other names:	Clenbuterol, trimethylsilyl ether Clenbuterol O-TMS
Inchi:	InChI=1S/C15H26Cl2N2OSi/c1-15(2,3)19-9-13(20-21(4,5)6)10-7-11(16)14(18)12(17)8-1
InchiKey:	SUUGLXIKEMNASC-UHFFFAOYSA-N
Formula:	C15H26Cl2N2OSi
SMILES:	CC(C)(C)NCC(O[Si](C)(C)C)c1cc(Cl)c(N)c(Cl)c1
Mol. weight [g/mol]:	349.37
CAS:	129138-61-0

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.11		Crippen Method
logp	4.856		Crippen Method
rinpol	1995.00		NIST Webbook
rinpol	1995.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C129138610&Units=SI

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/83-649-0/Clenbuterol-TMS-derivative.pdf>

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