

(.+/-)-Baclofen, N-(tert-butyldimethylsilyl)-, tert-butyldimethylsilyl ester

Other names:	(.+/-)-Baclofen, 2tdms derivative
Inchi:	InChI=1S/C22H40ClNO2Si2/c1-21(2,3)27(7,8)24-16-18(17-11-13-19(23)14-12-17)15-20
InchiKey:	OGFIJUGKNLYPBN-UHFFFAOYSA-N
Formula:	C22H40ClNO2Si2
SMILES:	CC(C)(C)[Si](C)(C)NCC(CC(=O)O[Si](C)(C)C(C)(C)C)c1ccc(Cl)cc1
Mol. weight [g/mol]:	442.18

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.94		Crippen Method
logp	6.957		Crippen Method
rinsol	2474.00		NIST Webbook
rinsol	2413.70		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=U333968&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/84-279-0/Baclofen-N-tert-butyldimethylsilyl-tert-butyldimethylsilyl-ester.pdf>

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