

7-Chloro-3-methyl-quinoline-8-carboxylic acid, tert-butyldimethylsilyl ester

Other names:	8-Quinolinecarboxylic acid, 7-chloro-3-methyl-, tert-butyldimethylsilyl- ether
Inchi:	InChI=1S/C17H22ClNO2Si/c1-11-9-12-7-8-13(18)14(15(12)19-10-11)16(20)21-22(5,6)17
InchiKey:	PQHBQAAWQOZUPV-UHFFFAOYSA-N
Formula:	C17H22ClNO2Si
SMILES:	<chem>Cc1cnc2c(C(=O)O[Si](C)(C)C(C)(C)C)c(Cl)ccc2c1</chem>
Mol. weight [g/mol]:	335.90

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	5.359		Crippen Method
rinpol	2310.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U373402&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws

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.cheméo.com/cid/33-036-5/7-Chloro-3-methyl-quinoline-8-carboxylic-acid-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-26 15:22:39.719197125 +0000 UTC m=+16434208.639774440.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.