

Quinaldic acid, tert-butyldimethylsilyl ester

Other names:	Quinaldic acid, tbdms derivative
Inchi:	InChI=1S/C16H21NO2Si/c1-16(2,3)20(4,5)19-15(18)14-11-10-12-8-6-7-9-13(12)17-14/h6
InchiKey:	ITGHOWDUPDGUJX-UHFFFAOYSA-N
Formula:	C16H21NO2Si
SMILES:	CC(C)(C)[Si](C)(C)OC(=O)c1ccc2ccccc2n1
Mol. weight [g/mol]:	287.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.43		Crippen Method
logp	4.397		Crippen Method
rinpol	2045.00		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=U352548&Units=SI

Legend

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

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<https://www.chemeo.com/cid/67-079-1/Quinaldic-acid-tert-butyldimethylsilyl-ester.pdf>

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