

3-Pyridinecarboxylic acid, trimethylsilyl ester

Other names:	Nicotinic acid-TMS Nicotinic acid, trimethylsilyl ester Trimethylsilyl nicotinate Niacin, tms derivative
Inchi:	InChI=1S/C9H13NO2Si/c1-13(2,3)12-9(11)8-5-4-6-10-7-8/h4-7H,1-3H3
InchiKey:	PYFBRRMHOWLGJH-UHFFFAOYSA-N
Formula:	C9H13NO2Si
SMILES:	C[Si](C)(C)OC(=O)c1cccnc1
Mol. weight [g/mol]:	195.29
CAS:	25436-37-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.37		Crippen Method
logp	2.073		Crippen Method
rinpol	1296.90		NIST Webbook
rinpol	1274.00		NIST Webbook
rinpol	1299.40		NIST Webbook
rinpol	1298.00		NIST Webbook
rinpol	1257.00		NIST Webbook
rinpol	1304.00		NIST Webbook
rinpol	1299.40		NIST Webbook
rinpol	1296.90		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25436377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/14-244-5/3-Pyridinecarboxylic-acid-trimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-26 19:04:40.116475945 +0000 UTC m=+16447529.037053260.

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