3-Pyridinimidic 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

Physical Properties

Property code	Value	Unit	Source
hf	-387.38	kJ/mol	Cheméo Relay (1.0)
hvap	63.74	kJ/mol	Cheméo Relay (1.0)
ie	9.56	eV	Cheméo Relay (1.0)
log10ws	-1.45		Cheméo Relay (1.0)
logp	2.073		Crippen Method
rinpol	1274.00		NIST Webbook
rinpol	1296.90		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
tb	510.42	K	Cheméo Relay (1.0)
tf	294.00	K	Cheméo Relay (1.0)

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C25436377&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):	

Legend

hf:	Enthalpy of formation at standard conditions
hvap:	Enthalpy of vaporization at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tf:	Normal melting (fusion) point