

N-METHYL NICOTINAMIDE TMS

Other names:	N-Methylnicotinamide, TMS
Inchi:	InChI=1S/C10H16N2OSi/c1-11-10(13-14(2,3)4)9-6-5-7-12-8-9/h5-8H,1-4H3
InchiKey:	DCVZXHVHFOITMY-UHFFFAOYSA-N
Formula:	C10H16N2OSi
SMILES:	CN=C(O[Si](C)(C)C)c1cccnc1
Mol. weight [g/mol]:	208.34

Physical Properties

Property code	Value	Unit	Source
hf	-186.94	kJ/mol	Cheméo Relay (1.0)
hvap	61.66	kJ/mol	Cheméo Relay (1.0)
ie	9.26	eV	Cheméo Relay (1.0)
log10ws	-1.09		Cheméo Relay (1.0)
logp	2.309		Crippen Method
rinpol	1431.00		NIST Webbook
tb	518.78	K	Cheméo Relay (1.0)
tf	282.76	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U141337&Units=SI>

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci990307I>

Crippen Method:

https://www.chemeo.com/doc/models/crippen_log10ws

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

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