1-Dimethyl(tert-butyl)silyloxy-4-nitrobenzene

Other names: 4-Nitrophenol, tert-butyldimethylsilyl ether
1-Dimethyl(tert-butyl)silyloxy-4-nitrobenzene
Inchi: InChI=1S/C12H19NO3Si/c1-12(2,3)17(4,5)16-11-8-6-10(7-9-11)13(14)15/h6-9H,1-5H3
InchiKey: AQPYYGDGBSMJJI-UHFFFAOYSA-N
Formula: C12H19NO3Si
SMILES: CC(C)(C)[Si](C)(C)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 253.37

Physical Properties

Property code	Value	Unit	Source
hf	-303.36	kJ/mol	Cheméo Relay (1.0)
ie	8.95	eV	Cheméo Relay (1.0)
log10ws	-3.93		Cheméo Relay (1.0)
logp	3.979		Crippen Method
rinpol	1784.40		NIST Webbook
rinpol	1732.00		NIST Webbook
tb	561.11	K	Cheméo Relay (1.0)
tf	408.02	K	Cheméo Relay (1.0)

Sources

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):
Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307925&Units=SI

Legend

hf: Enthalpy of formation 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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