4-Nitro-1-triisobutylsilyloxybenzene

Inchi: InChI=1S/C18H31NO3Si/c1-14(2)11-23(12-15(3)4,13-16(5)6)22-18-9-7-17(8-10-18)19(2
InchiKey: LNGZHORHHSXMET-UHFFFAOYSA-N
Formula: C18H31NO3Si
SMILES: CC(C)C[Si](CC(C)C)(CC(C)C)Oc1ccc([N+](=O)[O-])cc1
Mol. weight [g/mol]: 337.53

Physical Properties

Property code	Value	Unit	Source
hf	-409.84	kJ/mol	Cheméo Relay (1.0)
ie	8.85	eV	Cheméo Relay (1.0)
log10ws	-6.06		Cheméo Relay (1.0)
logp	5.887		Crippen Method
rinpol	2174.00		NIST Webbook
rinpol	2174.00		NIST Webbook
tb	617.32	K	Cheméo Relay (1.0)
tf	325.97	K	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0, beta):
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U307960&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
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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