Isovanilline, MO TMS

Inchi: InChI=1S/C12H19NO3Si/c1-14-11-7-6-10(9-13-15-2)8-12(11)16-17(3,4)5/h6-9H,1-5H3
InchiKey: XPJSIAMLVGTQRF-UHFFFAOYSA-N
Formula: C12H19NO3Si
SMILES: CON=Cc1ccc(OC)c(O[Si](C)(C)C)c1
Mol. weight [g/mol]: 253.37

Physical Properties

Property code	Value	Unit	Source
ie	8.05	eV	Cheméo Relay (1.0)
log10ws	-2.58		Cheméo Relay (1.0)
logp	2.889		Crippen Method
rinpol	1618.00		NIST Webbook
tb	567.67	K	Cheméo Relay (1.0)
tf	341.52	K	Cheméo Relay (1.0)

Sources

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=R92595&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

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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