Benzoic acid, 3-(tert.-butyldimethylsilyloxy)-, methyl ester

Inchi: InChI=1S/C14H22O3Si/c1-14(2,3)18(5,6)17-12-9-7-8-11(10-12)13(15)16-4/h7-10H,1-6H3

InchiKey: QTPQDOOFCLYBBG-UHFFFAOYSA-N

Formula: C14H22O3Si

SMILES: COC(=O)c1cccc(O[Si](C)(C)C(C)(C)C)c1

Mol. weight [g/mol]: 266.41

Physical Properties

Property code	Value	Unit	Source
af	0.6060		Cheméo Relay (1.0)
hf	-635.05	kJ/mol	Cheméo Relay (1.0)
hvap	71.39	kJ/mol	Cheméo Relay (1.0)
ie	8.65	eV	Cheméo Relay (1.0)
log10ws	-3.74		Cheméo Relay (1.0)
logp	3.857		Crippen Method
pc	1759.72	kPa	Cheméo Relay (1.0, beta)
rinpol	1691.00		NIST Webbook
rinpol	1691.00		NIST Webbook
tb	562.02	K	Cheméo Relay (1.0)
tc	775.69	K	Cheméo Relay (1.0)
tf	337.22	K	Cheméo Relay (1.0)
vc	0.803	m3/kmol	Cheméo Relay (1.0)

Sources

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U374358&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

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

Legend

af:	Acentric Factor
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
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume

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