Benzenepropanoic acid, alpha-oxo-beta, beta-bis(trimethylsilyl)-

Other names: Benzenepropanoic acid, «alpha»-oxo-, bis(trimethylsilyl)-
3-Hydroxycinnamic acid, di-TMS
Phenylpyruvic acid, bis-TMS

Inchi: InChI=1S/C15H24O3Si2/c1-19(2,3)17-14(15(16)18-20(4,5)6)12-13-10-8-7-9-11-13/h7-12

InchiKey: DUIQXZZFTOSCCA-WYMLVPIESA-N

Formula: C15H24O3Si2

SMILES: C[Si](C)(C)OC(=O)/C(=C/c1ccccc1)O[Si](C)(C)C

Mol. weight [g/mol]: 308.53

Physical Properties

Property code	Value	Unit	Source
ie	8.60	eV	Cheméo Relay (1.0)
logp	4.257		Crippen Method
tb	583.71	K	Cheméo Relay (1.0)
tf	289.06	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=C27750614&Units=SI

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient

tb: Normal Boiling Point Temperature

tf: Normal melting (fusion) point