Benzenepropanoic acid, «alpha»,4-bis[(trimethylsilyl)oxy]-, trimethylsilyl ester

Other names:	Hydrocinnamic acid, p,«alpha»-bis(trimethylsiloxy)-, trimethylsilyl ester
	4-Hydroxyphenyllactic acid, tris(trimethylsilyl) deriv.
	Trimethylsilyl 2-[(trimethylsilyl)oxy]-3-(4-[(trimethylsilyl)oxy]phenyl)propanoate
	4-Hydroxyphenyllactate, (3TMS)
	4-Hydroxyphenyllactic acid, tris-TMS
	4-Hydroxyphenyllactic acid, tri-TMS
	Phenyllactic acid, 4-hydroxy, (3TMS)
	Propanoic acid, 2-trimethylsilyloxy-3-(4-trimethylsilyloxyphenyl), trimethylsilyl ester
	Phenyllactic acid, 4-hydroxy, tri-TMS
	4-Hydroxyphenyllactate, TMS
	Phenyllactic acid, 4-hydroxy, TMS
	4-Hydroxyphenyllactic acid, diTMS
	4-Hydroxyphenyllactic acid, TMS
	4-Hydroxyphenyllactic acid, 3tms derivative
Inchi:	InChI=1S/C18H34O4Si3/c1-23(2,3)20-16-12-10-15(11-13-16)14-17(21-24(4,5)6)18(19)22
InchiKey:	ZSYIYFFJWIPCPN-UHFFFAOYSA-N
Formula:	C18H34O4Si3
SMILES:	C[Si](C)(C)OC(=O)C(Cc1ccc(O[Si](C)(C)C)cc1)O[Si](C)(C)C
Mol. weight [g/mol]:	398.72
CAS:	27750-67-0

Physical Properties

Property code	Value	Unit	Source
log10ws	1.62		Crippen Method
logp	5.041		Crippen Method
rinpol	1912.00		NIST Webbook
rinpol	1894.00		NIST Webbook
rinpol	1907.00		NIST Webbook
rinpol	1910.00		NIST Webbook
rinpol	1920.00		NIST Webbook
rinpol	1908.00		NIST Webbook
rinpol	1921.00		NIST Webbook
rinpol	1909.00		NIST Webbook
rinpol	1912.00		NIST Webbook
rinpol	1919.00		NIST Webbook
rinpol	1906.00		NIST Webbook
rinpol	1935.00		NIST Webbook

rinpol	1923.00	NIST Webbook
rinpol	1919.00	NIST Webbook
rinpol	1910.00	NIST Webbook
rinpol	1912.00	NIST Webbook
rinpol	1906.00	NIST Webbook
rinpol	1935.00	NIST Webbook
rinpol	1928.00	NIST Webbook
rinpol	1919.00	NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750670&Units=SI

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

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

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices