2,5-Dimethoxycinnamic acid, tert-butyldimethylsilyl ester

Other names: 2,5-Dimethoxycinnamic acid, TBDMS
Inchi: InChI=1S/C17H26O4Si/c1-17(2,3)22(6,7)21-16(18)11-8-13-12-14(19-4)9-10-15(13)20-5/
InchiKey: CJHKJVRLGCHXQN-DHZHZOJOSA-N
Formula: C17H26O4Si
SMILES: COc1ccc(OC)c(C=CC(=O)O[Si](C)(C)C(C)(C)C)c1
Mol. weight [g/mol]: 322.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.20		Cheméo Relay (1.0)
logp	4.265		Crippen Method
rinpol	2241.00		NIST Webbook
rinpol	2241.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U364359&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):
Cheméo Relay (1.0, beta):

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices

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