

Ferulic acid, tert-butyldimethylsilyl ether, tert-butyldimethylsilyl ester

Other names:

Ferulic acid, TBDMS

Ferulic acid, 2tdms derivative

Inchi:

InChI=1S/C22H38O4Si2/c1-21(2,3)27(8,9)25-18-14-12-17(16-19(18)24-7)13-15-20(23)2

InchiKey:

XHLCLAOSZFRAJG-FYWRMAATSA-N

Formula:

C22H38O4Si2

SMILES:

COc1cc(C=CC(=O)O[Si](C)(C)C(C)(C)C)ccc1O[Si](C)(C)C(C)(C)C

Mol. weight [g/mol]:

422.71

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.52		Crippen Method
logp	6.641		Crippen Method
rinpol	2597.10		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2612.00		NIST Webbook
rinpol	2597.10		NIST Webbook

Sources

Crippen Method:

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Crippen Method:

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

NIST Webbook:

<http://webbook.nist.gov/cgi/cbook.cgi?ID=U352565&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/38-216-0/Ferulic-acid-tert-butyldimethylsilyl-ether-tert-butyldimethylsilyl-ester.pdf>

Generated by Cheméo on 2024-04-20 12:39:13.90080647 +0000 UTC m=+15906002.821383780.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.