

2-Methoxycinnamic acid, trimethylsilyl ester

Other names:	2-Methoxycinnamic acid, tms derivative
Inchi:	InChI=1S/C13H18O3Si/c1-15-12-8-6-5-7-11(12)9-10-13(14)16-17(2,3)4/h5-10H,1-4H3/b
InchiKey:	IREWBZSPSFACTL-MDZDMXLPSA-N
Formula:	C13H18O3Si
SMILES:	COc1ccccc1C=CC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	250.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.00		Crippen Method
logp	3.086		Crippen Method
rinpol	1757.00		NIST Webbook
rinpol	1788.50		NIST Webbook
rinpol	1788.50		NIST Webbook
rinpol	1757.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U352482&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071

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/122-917-8/2-Methoxycinnamic-acid-trimethylsilyl-ester.pdf>

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