

4-Methoxyphenylpropionic acid trimethylsilyl ester

Other names:

4-Methoxyphenylpropionic acid, TMS
Trimethylsilyl 3-(4-methoxyphenyl)propanoate
Benzenepropanoic acid, 4-methoxy, TMS
3-(4-Methoxyphenyl)propionic acid, tms derivative

Inchi: InChI=1S/C13H20O3Si/c1-15-12-8-5-11(6-9-12)7-10-13(14)16-17(2,3)4/h5-6,8-9H,7,10H

InchiKey: YDYQZJMNZRCJOR-UHFFFAOYSA-N

Formula: C13H20O3Si

SMILES: COc1ccc(CCC(=O)O[Si](C)(C)C)cc1

Mol. weight [g/mol]: 252.38

CAS: 27750-58-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	3.006		Crippen Method
rinpol	1643.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750589&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

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<https://www.chemeo.com/cid/63-321-5/4-Methoxyphenylpropionic-acid-trimethylsilyl-ester.pdf>

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