

2-Methoxyphenylpropionic acid, trimethylsilyl ester

Other names:

(2-Methoxyphenyl)propionic acid, TMS
Trimethylsilyl 3-(2-methoxyphenyl)propanoate
Hydrocinnamic acid, o-methoxy-, trimethylsilyl ester
Benzenepropanoic acid, 2-methoxy, trimethylsilyl ester
3-(2-Methoxyphenyl)propanoic acid, tms derivative

Inchi: InChI=1S/C13H20O3Si/c1-15-12-8-6-5-7-11(12)9-10-13(14)16-17(2,3)4/h5-8H,9-10H2,1

InchiKey: DCZUUHAXBALCCL-UHFFFAOYSA-N

Formula: C13H20O3Si

SMILES: COc1ccccc1CCC(=O)O[Si](C)(C)C

Mol. weight [g/mol]: 252.38

CAS: 27750-54-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.98		Crippen Method
logp	3.006		Crippen Method
rinpol	1595.00		NIST Webbook
rinpol	1595.00		NIST Webbook

Sources

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

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C27750545&Units=SI>

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

Legend

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

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