Phenylethylmalonic acid, bis(trimethylsilyl) ester

Other names: Phenylethylmalonic acid, di-TMS
Inchi: InChI=1S/C17H28O4Si2/c1-8-17(14-12-10-9-11-13-14,15(18)20-22(2,3)4)16(19)21-23(5,
InchiKey: XZKIYKRYUAODMJ-UHFFFAOYSA-N
Formula: C17H28O4Si2
SMILES: CCC(C(=O)O[Si](C)(C)C)(C(=O)O[Si](C)(C)C)c1ccccc1
Mol. weight [g/mol]: 352.57
CAS: 55517-51-6

Physical Properties

Property code	Value	Unit	Source
log10ws	0.46		Crippen Method
logp	4.091		Crippen Method
rinpol	1700.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1700.00		NIST Webbook

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517516&Units=SI

Legend

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

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