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]: 352.58

Physical Properties

Property code	Value	Unit	Source
logp	4.091		Crippen Method
rinpol	1700.00		NIST Webbook
rinpol	1725.00		NIST Webbook
rinpol	1700.00		NIST Webbook
tf	347.31	K	Cheméo Relay (1.0)

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C55517516&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
Cheméo Relay (1.0):
Cheméo Relay (1.0, beta):

Legend

logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices
tf: Normal melting (fusion) point