Adipic acid, trimethylsilyl ester

Other names:	6-Oxo-6-[(trimethylsilyl)oxy]hexanoic acid
	Adipic acid, tms derivative
Inchi:	InChI=1S/C9H18O4Si/c1-14(2,3)13-9(12)7-5-4-6-8(10)11/h4-7H2,1-3H3,(H,10,11)
InchiKey:	NXRUXRPNYSMFBT-UHFFFAOYSA-N
Formula:	C9H18O4Si
SMILES:	C[Si](C)(C)OC(=O)CCCCC(=O)O
Mol. weight [g/mol]:	218.32

Physical Properties

Property code	Value	Unit	Source
log10ws	0.40		Crippen Method
logp	2.010		Crippen Method
rinpol	1413.10		NIST Webbook
rinpol	1413.10		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=U332809&Units=SI

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/43-586-4/Adipic-acid-trimethylsilyl-ester.pdf
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