Heptanoic acid, tert-butyldimethylsilanyl ester

Other names:	Heptanoic acid, tert-butyldimethylsilyl ester
	tert-Butyl(dimethyl)silyl heptanoate
	Heptanoic acid, DMTBS
	Heptanoic acid, TBDMS
	Heptanoic acid, tbdms derivative
Inchi:	InChI=1S/C13H28O2Si/c1-7-8-9-10-11-12(14)15-16(5,6)13(2,3)4/h7-11H2,1-6H3
InchiKey:	RHWPBALXGUQVAC-UHFFFAOYSA-N
Formula:	C13H28O2Si
SMILES:	CCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	244.45
CAS:	54251-63-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.18		Crippen Method
logp	4.505		Crippen Method
rinpol	1383.10		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1378.00		NIST Webbook
rinpol	1389.00		NIST Webbook
rinpol	1388.00		NIST Webbook
rinpol	1383.10		NIST Webbook
ripol	1474.00		NIST Webbook
ripol	1474.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C54251637&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

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

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