Hexanoic acid, tert-butyldimethylsilyl ester

Other names:	tert-Butyl(dimethyl)silyl hexanoate
	Hexanoic acid, DMTBS
	Hexanoic acid, TBDMS
	Caproic acid, DMTBS
	Caproic acid, TBDMS
	Hexanoic acid, tbdms derivative
Inchi:	InChI=1S/C12H26O2Si/c1-7-8-9-10-11(13)14-15(5,6)12(2,3)4/h7-10H2,1-6H3
InchiKey:	SSUYOKULCCIOEK-UHFFFAOYSA-N
Formula:	C12H26O2Si
SMILES:	CCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	230.42

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.76		Crippen Method
logp	4.115		Crippen Method
rinpol	1286.00		NIST Webbook
rinpol	1276.00		NIST Webbook
rinpol	1291.00		NIST Webbook
rinpol	1283.00		NIST Webbook
rinpol	1294.00		NIST Webbook
rinpol	1290.00		NIST Webbook
ripol	1385.00		NIST Webbook
ripol	1385.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333118&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
ripol:	Polar retention indices

Latest version available from:

https://www.chemeo.com/cid/54-104-6/Hexanoic-acid-tert-butyldimethylsilyl-ester.pdf

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