

Octanoic acid, tert-butyldimethylsilyl ester

Other names:	Octanoic acid, DMTBS Octanoic acid, TBDMS Caprylic acid, TBDMS Caprylic acid, DMTBS tert-Butyl(dimethyl)silyl octanoate Octanoic acid, tbdms derivative
Inchi:	InChI=1S/C14H30O2Si/c1-7-8-9-10-11-12-13(15)16-17(5,6)14(2,3)4/h7-12H2,1-6H3
InchiKey:	FLZPUMRVXOBSIN-UHFFFAOYSA-N
Formula:	C14H30O2Si
SMILES:	CCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	258.47
CAS:	104255-72-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.60		Crippen Method
logp	4.895		Crippen Method
rinpol	1487.70		NIST Webbook
rinpol	1482.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1465.00		NIST Webbook
rinpol	1446.00		NIST Webbook
rinpol	1487.70		NIST Webbook
rinpol	1486.00		NIST Webbook
ripol	1582.00		NIST Webbook
ripol	1582.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255723&Units=SI>

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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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