

Dodecanoic acid, tert-butyldimethylsilyl ester

Other names: Dodecanoic acid, DMTBS
Dodecanoic acid, TBDMS
Lauric acid, DMTBS
Lauric acid, TBDMS
Dodecanoic acid, tbdms derivative

Inchi: InChI=1S/C18H38O2Si/c1-7-8-9-10-11-12-13-14-15-16-17(19)20-21(5,6)18(2,3)4/h7-16H

InchiKey: BXOQPDP LCKIVSL-UHFFFAOYSA-N

Formula: C18H38O2Si

SMILES: CCCCCCCCCC(=O)O[Si](C)(C)C(C)C

Mol. weight [g/mol]: 314.58

CAS: 104255-77-8

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.27		Crippen Method
logp	6.456		Crippen Method
rinpol	1881.40		NIST Webbook
rinpol	1872.00		NIST Webbook
rinpol	1884.00		NIST Webbook
rinpol	1874.00		NIST Webbook
rinpol	1881.40		NIST Webbook
rinpol	1884.00		NIST Webbook
ripol	1977.00		NIST Webbook
ripol	1977.00		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=C104255778&Units=SI>

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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