

Dodecanoic acid, trimethylsilyl ester

Other names:	Trimethylsilyl laurate Dodecanoic acid, TMS ester Lauric acid (TMS) Lauric acid, trimethylsilyl ester Dodecanoic acid, tms derivative
Inchi:	InChI=1S/C15H32O2Si/c1-5-6-7-8-9-10-11-12-13-14-15(16)17-18(2,3)4/h5-14H2,1-4H3
InchiKey:	RHDZBWSXEZTMPK-UHFFFAOYSA-N
Formula:	C15H32O2Si
SMILES:	CCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]:	272.50
CAS:	55520-95-1

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.01		Crippen Method
logp	5.285		Crippen Method
rinpol	1643.10		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1648.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1650.00		NIST Webbook
rinpol	1651.70		NIST Webbook
rinpol	1645.20		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1647.00		NIST Webbook
rinpol	1651.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1657.00		NIST Webbook
rinpol	1654.00		NIST Webbook
rinpol	1662.00		NIST Webbook
rinpol	1657.00		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=C55520951&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/39-451-8/Dodecanoic-acid-trimethylsilyl-ester.pdf>

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