

Pentadecanoic acid, tert-butyldimethylsilyl ester

Other names:	Pentadecanoic acid, TBDMS Pentadecanoic acid, DMTBS tert-Butyl(dimethyl)silyl pentadecanoate Pentadecanoic acid, tbdms derivative
Inchi:	InChI=1S/C21H44O2Si/c1-7-8-9-10-11-12-13-14-15-16-17-18-19-20(22)23-24(5,6)21(2,3
InchiKey:	DHOAONBYKUBKBP-UHFFFAOYSA-N
Formula:	C21H44O2Si
SMILES:	CCCCCCCCCCCCCCC(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]:	356.66
CAS:	104255-80-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.53		Crippen Method
logp	7.626		Crippen Method
rinpol	2185.00		NIST Webbook
rinpol	2181.20		NIST Webbook
rinpol	2184.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2174.00		NIST Webbook
rinpol	2185.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C104255803&Units=SI

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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