

Isoheptadecanoic acid, TMS

Inchi: InChI=1S/C20H42O2Si/c1-19(2)17-15-13-11-9-7-6-8-10-12-14-16-18-20(21)22-23(3,4)5/
InchiKey: BWAZLAVYOIAGHB-UHFFFAOYSA-N
Formula: C20H42O2Si
SMILES: CC(C)CCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 342.63

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.87		Crippen Method
logp	7.092		Crippen Method
rinpol	2120.00		NIST Webbook
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Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R573594&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

Latest version available from:

<https://www.chemeo.com/cid/34-339-8/Isoheptadecanoic-acid-TMS.pdf>

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