

Isononadecanoic acid, TMS

Inchi: InChI=1S/C22H46O2Si/c1-21(2)19-17-15-13-11-9-7-6-8-10-12-14-16-18-20-22(23)24-25
InchiKey: CHKQVJYRLNSJTF-UHFFFAOYSA-N
Formula: C22H46O2Si
SMILES: CC(C)CCCCCCCCCCCCCCC(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 370.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.70		Crippen Method
logp	7.872		Crippen Method
rinsol	2320.00		NIST Webbook
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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=R573603&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinsol: Non-polar retention indices

Latest version available from:

<https://www.chemeo.com/cid/34-213-7/Isononadecanoic-acid-TMS.pdf>

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