

Dodecanoic acid, 2-hydroxy, DTBS

Inchi: InChI=1S/C20H40O3Si/c1-8-9-10-11-12-13-14-15-16-17-18(21)23-24(22-17,19(2,3)4)20
InchiKey: XMCYXEHALCBNOE-UHFFFAOYSA-N
Formula: C20H40O3Si
SMILES: CCCCCCCCCC1O[Si](C(C)(C)C)(C(C)(C)C)OC1=O
Mol. weight [g/mol]: 356.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.78		Crippen Method
logp	6.502		Crippen Method
rinpol	2175.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R115361&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/87-300-2/Dodecanoic-acid-2-hydroxy-DTBS.pdf>

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