

Dodecanoic acid, bromomethyl dimethylsilyl ester

Inchi: InChI=1S/C15H31BrO2Si/c1-4-5-6-7-8-9-10-11-12-13-15(17)18-19(2,3)14-16/h4-14H2,1
InchiKey: XWKNMBKHQDNTNI-UHFFFAOYSA-N
Formula: C15H31BrO2Si
SMILES: CCCCCCCCCCCC(=O)O[Si](C)(C)CBr
Mol. weight [g/mol]: 351.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.53		Crippen Method
logp	5.590		Crippen Method
rinpol	1969.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U375511&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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<https://www.cheméo.com/cid/75-165-6/Dodecanoic-acid-bromomethyl-dimethylsilyl-ester.pdf>

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