

2-Furancarboxylic acid, 5-[[trimethylsilyloxy]methyl]-, trimethylsilyl ester

Other names:
ester

5-Trimethylsiloxymethyl-2-trimethylsilylfuroate

2-Furoic acid, 5-hydroxymethyl, bis-TMS

2-Hydroxymethylfuran-5-carboxylic acid, di-TMS

2-Furoic acid, 5-hydroxymethyl, TMS

5-Hydroxymethyl-2-furoic acid, 2tms derivative

Inchi:

InChI=1S/C12H22O4Si2/c1-17(2,3)14-9-10-7-8-11(15-10)12(13)16-18(4,5)6/h7-8H,9H2,

InchiKey:

XHRIJDKBFZGXAB-UHFFFAOYSA-N

Formula:

C12H22O4Si2

SMILES:

C[Si](C)(C)OCc1ccc(C(=O)O[Si](C)(C)C)o1

Mol. weight [g/mol]:

286.47

CAS:

55517-40-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Crippen Method
logp	3.623		Crippen Method
rinpol	1540.00		NIST Webbook
rinpol	1560.00		NIST Webbook
rinpol	1561.00		NIST Webbook
rinpol	1540.00		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=C55517403&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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