

2,4-Imidazolidinedione, 5,5-diphenyl-1,3-bis(trimethylsilyl)-

Other names:

Bis(trimethylsilyl) derivative of Phenytoin

N,N-Bis(trimethylsilyl)-diphenylhydantoin

5,5-Diphenylhydantoin, N,N'-bis(trimethylsilyl)-

Phenytoin, 2tms derivative

Inchi:

InChI=1S/C21H28N2O2Si2/c1-26(2,3)22-19(24)21(17-13-9-7-10-14-17,18-15-11-8-12-16

InchiKey:

FBXVMNWJCVYLIN-UHFFFAOYSA-N

Formula:

C₂₁H₂₈N₂O₂Si₂

SMILES:

C[Si](C)(C)N1C(=O)N([Si](C)(C)C)C(c2ccccc2)(c2ccccc2)C1=O

Mol. weight [g/mol]:

396.63

CAS:

63435-72-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-0.75		Crippen Method
logp	4.864		Crippen Method
rinpol	2272.90		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=C63435723&Units=SI>

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/39-949-6/2-4-Imidazolidinedione-5-5-diphenyl-1-3-bis-trimethylsilyl.pdf>

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