

4-Hydroxycoumarin, tert-butyldimethylsilyl ether

Other names:	4-Pyrrol[tert-butyl(dimethyl)silyl]oxymorpho-2H-chromen-2-one 4-Hydroxycoumarin, tbdms derivative
Inchi:	InChI=1S/C15H20O3Si/c1-15(2,3)19(4,5)18-13-10-14(16)17-12-9-7-6-8-11(12)13/h6-10H
InchiKey:	QFEJYZZDRJQHGP-UHFFFAOYSA-N
Formula:	C15H20O3Si
SMILES:	CC(C)(C)[Si](C)(C)Oc1cc(=O)oc2ccccc12
Mol. weight [g/mol]:	276.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.70		Crippen Method
logp	4.177		Crippen Method
rinpol	2140.50		NIST Webbook
rinpol	2141.30		NIST Webbook
rinpol	2140.50		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U333103&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/47-226-9/4-Hydroxycoumarin-tert-butyldimethylsilyl-ether.pdf>

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