6,7-Dihydroxycoumarin, bis(trimethylsilyl) ether

Other names: Coumarin, 6,7-dihydroxy-, TMS
Aesculetin, TMS
Coumarin, 6,7-bis-trimethylsilyloxy

Inchi: InChI=1S/C15H22O4Si2/c1-20(2,3)18-13-9-11-7-8-15(16)17-12(11)10-14(13)19-21(4,5)6

InchiKey: KATLNZVTBBAXMH-UHFFFAOYSA-N

Formula: C15H22O4Si2

SMILES: C[Si](C)(C)Oc1cc2ccc(=O)oc2cc1O[Si](C)(C)C

Mol. weight [g/mol]: 322.50

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.45		Crippen Method
logp	4.220		Crippen Method
rinpol	2125.00		NIST Webbook
rinpol	2125.00		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=U108963&Units=SI

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

Cheméo (https://www.chemeo.com) is the biggest free database of chemical and physical data for the process industry.