9,10-Anthracenedione, 3-methyl-1,6,8-tris[(trimethylsilyl)oxy]-

Other names:	3-Methyl-1,6,8-tris[(trimethylsilyl)oxy]anthra-9,10-quinone
	Anthraquinone, 1,3,8-trihydroxy-6-methyl, tris-TMS
	Anthraquinone, 1,6,8-tris-hydroxy-3-methyl, tris-TMS
	Emodin, tri-TMS
	Anthraquinone, 1,3,8-trihydroxy-6-methyl, TMS
	Emodin, TMS
	Anthraquinone, 1,6,8-tris-hydroxy-3-methyl, TMS
	Emodin, 3tms derivative
Inchi:	InChI=1S/C24H34O5Si3/c1-15-11-17-21(19(12-15)28-31(5,6)7)24(26)22-18(23(17)25)13
InchiKey:	AJHJEZGOTQJNSB-UHFFFAOYSA-N
Formula:	C24H34O5Si3
SMILES:	Cc1cc(O[Si](C)(C)C)c2c(c1)C(=O)c1cc(O[Si](C)(C)C)cc(O[Si](C)(C)C)c1C2=O
Mol. weight [g/mol]:	486.78
CAS:	7336-74-5

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.13		Crippen Method
logp	6.412		Crippen Method
rinpol	2883.00		NIST Webbook
rinpol	2883.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7336745&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