1,8-Dihydroxy-3-methylanthraquinone, O,O'-bis(trimethylsilyl-)

Other names:	3-Methyl-1,8-bis[(trimethylsilyl)oxy]anthra-9,10-quinone
	Anthraquinone, 1,8-dihydroxy-3-methyl, bis-TMS
	Chrysophanol, bis-TMS
	Chrysophanol, TMS
	Anthraquinone, 1,8-dihydroxy-3-methyl, TMS
	Chrysophanol, 2tms derivative
Inchi:	InChI=1S/C21H26O4Si2/c1-13-11-15-19(17(12-13)25-27(5,6)7)21(23)18-14(20(15)22)9-
InchiKey:	BJOOPYSIRYXVDH-UHFFFAOYSA-N
Formula:	C21H26O4Si2
SMILES:	Cc1cc(O[Si](C)(C)C)c2c(c1)C(=O)c1cccc(O[Si](C)(C)C)c1C2=O
Mol. weight [g/mol]:	398.60
CAS:	7336-72-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.12		Crippen Method
logp	5.198		Crippen Method
rinpol	2612.00		NIST Webbook

Sources

Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C7336723&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
rinpol:	Non-polar retention indices