

1,8-Dihydroxy-6-methoxy-3-methylanthraquinone

Other names: 3-Methoxy-6-methyl-1,8-bis[(trimethylsilyl)oxy]anthra-9,10-quinone
O,O'-bis(trimethylsilyl)

Anthraquinone, 1,8-dihydroxy-6-methoxy-3-methyl, bis-TMS

Anthraquinone, 1,8-dihydroxy-6-methoxy-3-methyl, TMS

Physcion, TMS

Inchi: InChI=1S/C22H28O5Si2/c1-13-9-15-19(17(10-13)26-28(3,4)5)22(24)20-16(21(15)23)11-

InchiKey: KTQHHXYXDHXNHO-UHFFFAOYSA-N

Formula: C22H28O5Si2

SMILES: COc1cc(O[Si](C)(C)C)c2c(c1)C(=O)c1cc(C)cc(O[Si](C)(C)C)c1C2=O

Mol. weight [g/mol]: 428.63

CAS: 7336-75-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	5.206		Crippen Method
rinpol	2836.00		NIST Webbook
rinpol	2836.00		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=C7336756&Units=SI>

Legend

log10ws: Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

rinpol: Non-polar retention indices

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