

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

Other names: Anthraquinone, 1,6-dihydroxy-8-methoxy-3-methyl, (2TMS)-
O,O'-bis(trimethylsilyl)-Anthraquinone, 1,6-dihydroxy-8-methoxy-3-methyl, TMS

Questin, TMS

Inchi: InChI=1S/C22H28O5Si2/c1-13-9-15-20(18(10-13)27-29(6,7)8)22(24)19-16(21(15)23)11-

InchiKey: PMYLCIIIYAHNIC-UHFFFAOYSA-N

Formula: C22H28O5Si2

SMILES: COc1cc(O[Si](C)(C)C)cc2c1C(=O)c1c(O[Si](C)(C)C)cc(C)cc1C2=O

Mol. weight [g/mol]: 428.63

CAS: 91701-23-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.24		Crippen Method
logp	5.206		Crippen Method
rinpol	2846.00		NIST Webbook
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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=C91701234&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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