

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

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