

Chrysophanol-9-anthrone, TMS

Inchi: InChI=1S/C21H28O3Si2/c1-14-11-16-13-15-9-8-10-17(23-25(2,3)4)19(15)21(22)20(16)1
InchiKey: VYMALBZKMBEIHU-UHFFFAOYSA-N
Formula: C₂₁H₂₈O₃Si₂
SMILES: Cc1cc2c(c(O[Si](C)(C)C)c1)C(=O)c1c(cccc1O[Si](C)(C)C)C2
Mol. weight [g/mol]: 384.62

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.27		Crippen Method
logp	5.558		Crippen Method
rinpol	2452.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158204&Units=SI>

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/57-611-0/Chrysophanol-9-anthrone-TMS.pdf>

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