

Obtusin, TMS

Inchi: InChI=1S/C24H32O7Si2/c1-13-11-14-17(23(29-4)21(13)30-32(5,6)7)20(26)18-15(19(14))
InchiKey: PDKPQQCHHOQIMO-UHFFFAOYSA-N
Formula: C24H32O7Si2
SMILES: COc1cc2c(c(O[Si](C)(C)C)c1OC)C(=O)c1c(cc(C)c(O[Si](C)(C)C)c1OC)C2=O
Mol. weight [g/mol]: 488.68

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Crippen Method
logp	5.224		Crippen Method
rinpol	3080.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R158279&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.chemeo.com/cid/58-364-4/Obtusin-TMS.pdf>

Generated by Cheméo on 2025-12-05 23:32:26.774678492 +0000 UTC m=+4725744.304719234.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.