

Tropate, TMS

Inchi: InChI=1S/C20H29NO4Si/c1-21-16-10-14(11-17(21)19-18(16)25-19)24-20(22)15(12-23-2
InchiKey: KYAGWQUTVDHVGQ-XTFZJFRFSA-N
Formula: C20H29NO4Si
SMILES: CN1C2CC(OC(=O)C(CO[Si](C)(C)C)c3ccccc3)CC1C1OC12
Mol. weight [g/mol]: 375.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-1.16		Crippen Method
logp	2.777		Crippen Method
rinpol	1599.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R330560&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/41-810-6/Tropate-TMS.pdf>

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