

Bilobalide, TMS ether

Inchi: InChI=1S/C21H34O8Si2/c1-18(2,3)20(29-31(7,8)9)10-12-19(11-13(22)25-12)16(24)27-1
InchiKey: JOLOPTLRBSAWFO-UHFFFAOYSA-N
Formula: C₂₁H₃₄O₈Si₂
SMILES: CC(C)(C)C1(O[Si](C)(C)C)CC2OC(=O)CC23C(=O)OC2OC(=O)C(O[Si](C)(C)C)C231
Mol. weight [g/mol]: 470.66
CAS: 480427-37-0

Physical Properties

Property code	Value	Unit	Source
log10ws	0.73		Crippen Method
logp	2.975		Crippen Method
rinpola	2481.90		NIST Webbook
rinpola	2504.20		NIST Webbook
rinpola	2526.70		NIST Webbook
rinpola	2438.30		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=C480427370&Units=SI>

Legend

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

Latest version available from:

<https://www.chemeo.com/cid/77-505-6/Bilobalide-TMS-ether.pdf>

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