

Redbank ketol, TMS

Inchi: InChI=1S/C18H30O3Si/c1-13(2)10-18(21-22(4,5)6)11-14(3)9-16(18)17(19)15-7-8-20-12-
InchiKey: ZCCISJKRESRHP-ZVZYQTTQSA-N
Formula: C18H30O3Si
SMILES: CC(C)CC1(O[Si](C)(C)C)CC(C)CC1C(=O)c1ccoc1
Mol. weight [g/mol]: 322.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.31		Crippen Method
logp	5.145		Crippen Method
rinpol	1779.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R584846&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/27-817-5/Redbank-ketol-TMS.pdf>

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