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:	ZCCISJKRESPRHP-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

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R584846&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

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

Generated by Cheméo on 2024-10-12 06:57:11.894368506 +0000 UTC m=+3297094.531337764.

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