

Succinylacetone, O-pentafluorobenzoyloxime, TMS

Inchi: InChI=1S/C24H22F10N2O4Si/c1-10(35-38-8-12-15(25)19(29)23(33)20(30)16(12)26)7-11
InchiKey: SYVIKTYZHWOGPK-OZQSKDJKSA-N
Formula: C24H22F10N2O4Si
SMILES: CC(CC(CCC(=O)O[Si](C)(C)C)=NOCc1c(F)c(F)c(F)c(F)c1F)=NOCc1c(F)c(F)c(F)c(F)c1F
Mol. weight [g/mol]: 620.51

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.78		Crippen Method
logp	7.091		Crippen Method
rinpola	2434.00		NIST Webbook
rinpola	2446.00		NIST Webbook
rinpola	2461.00		NIST Webbook
rinpola	2497.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R315378&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.cheméo.com/cid/33-071-6/Succinylacetone-O-pentafluorobenzoyloxime-TMS.pdf>

Generated by Cheméo on 2024-04-24 16:28:21.40919815 +0000 UTC m=+16265350.329775466.

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