

Octanoic acid, 2-oxo, O-pentafluorobenzoyloxime, TMS

Inchi: InChI=1S/C18H24F5NO3Si/c1-5-6-7-8-9-12(18(25)27-28(2,3)4)24-26-10-11-13(19)15(21)
InchiKey: TWUWJVJBGARBPJ-WY MPLXKRSA-N
Formula: C18H24F5NO3Si
SMILES: CCCCCC(=NOCc1c(F)c(F)c(F)c(F)c1F)C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 425.47

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.77		Crippen Method
logp	5.603		Crippen Method
rinpol	1837.00		NIST Webbook
rinpol	1837.00		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R315487&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/117-163-1/Octanoic-acid-2-oxo-O-pentafluorobenzoyloxime-TMS.pdf>

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