

Benzoic acid, 2-heptyl-6-hydroxy- 9 (2TMS)

Inchi: InChI=1S/C20H36O3Si2/c1-8-9-10-11-12-14-17-15-13-16-18(22-24(2,3)4)19(17)20(21)2
InchiKey: OZSNYLACMKGYCN-UHFFFAOYSA-N
Formula: C20H36O3Si2
SMILES: CCCCCCc1ccc(O[Si](C)(C)C)c1C(=O)O[Si](C)(C)C
Mol. weight [g/mol]: 380.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.51		Crippen Method
logp	6.405		Crippen Method
rinpol	2053.30		NIST Webbook
rinpol	2053.30		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=U414109&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.cheméo.com/doc/models/crippen_log10ws

Legend

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

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<https://www.cheméo.com/cid/117-594-3/Benzoic-acid-2-heptyl-6-hydroxy-9-2TMS.pdf>

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