

Fenoprofen, TBDMS

Inchi: InChI=1S/C21H28O3Si/c1-16(20(22)24-25(5,6)21(2,3)4)18-14-10-11-15-19(18)23-17-12
InchiKey: RTOVOPCSPWPMLK-UHFFFAOYSA-N
Formula: C21H28O3Si
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccccc1Oc1ccccc1
Mol. weight [g/mol]: 356.53

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.72		Crippen Method
logp	6.131		Crippen Method
rinpol	2239.90		NIST Webbook
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Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258567&Units=SI>

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/14-210-2/Fenoprofen-TBDMS.pdf>

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