

Flurbiprofen, TBDMS

Inchi: InChI=1S/C21H27FO2Si/c1-15(20(23)24-25(5,6)21(2,3)4)17-12-13-18(19(22)14-17)16-1
InchiKey: QFSTUWGNRAEVQW-UHFFFAOYSA-N
Formula: C21H27FO2Si
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccc(-c2ccccc2)c(F)c1
Mol. weight [g/mol]: 358.52

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.02		Crippen Method
logp	6.145		Crippen Method
rinpol	2269.20		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258601&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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/46-374-6/Flurbiprofen-TBDMS.pdf>

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