

Niflumic acid, ethoxycarbonylated, TBDMS

Inchi: InChI=1S/C22H27F3N2O4Si/c1-7-30-20(29)27(16-11-8-10-15(14-16)22(23,24)25)18-17(26)
InchiKey: WQPHZPQPYSFKPU-UHFFFAOYSA-N
Formula: C22H27F3N2O4Si
SMILES: CCOC(=O)N(c1cccc(C(F)(F)F)c1)c1cccc1C(=O)O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 468.54

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.11		Crippen Method
logp	6.557		Crippen Method
rinpol	2328.00		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R564664&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/61-756-5/Niflumic-acid-ethoxycarbonylated-TBDMS.pdf>

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