

Indoprofen, TBDMS

Inchi: InChI=1S/C23H29NO3Si/c1-16(22(26)27-28(5,6)23(2,3)4)17-11-13-19(14-12-17)24-15-1
InchiKey: ROUCAAPISJNOKA-UHFFFAOYSA-N
Formula: C23H29NO3Si
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccc(N2Cc3ccccc3C2=O)cc1
Mol. weight [g/mol]: 395.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.31		Crippen Method
logp	5.499		Crippen Method
rinpol	3110.30		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258621&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

Latest version available from:

<https://www.cheméo.com/cid/43-582-8/Indoprofen-TBDMS.pdf>

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