

Alclofenac, TBDMS

Inchi: InChI=1S/C17H25ClO3Si/c1-7-10-20-15-9-8-13(11-14(15)18)12-16(19)21-22(5,6)17(2,3)
InchiKey: ZDVORYVUQJYAMM-UHFFFAOYSA-N
Formula: C17H25ClO3Si
SMILES: C=CCOc1ccc(CC(=O)O[Si](C)(C)C(C)(C)C)cc1Cl
Mol. weight [g/mol]: 340.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.20		Crippen Method
logp	4.996		Crippen Method
rinpol	2103.00		NIST Webbook
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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=R258527&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/113-401-0/Alclofenac-TBDMS.pdf>

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