

Zomepirac, TBDMS

Inchi: InChI=1S/C21H28ClNO3Si/c1-14-12-17(13-18(24)26-27(6,7)21(2,3)4)23(5)19(14)20(25)
InchiKey: OMRIDVYXBKBWNC-UHFFFAOYSA-N
Formula: C21H28ClNO3Si
SMILES: Cc1cc(CC(=O)O[Si](C)(C)C(C)(C)C)n(C)c1C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 405.99

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.11		Crippen Method
logp	5.309		Crippen Method
rinsol	2729.10		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258745&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
rinsol: Non-polar retention indices

Latest version available from:

<https://www.cheméo.com/cid/96-350-7/Zomepirac-TBDMS.pdf>

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