

Fentiazac, TBDMS

Inchi: InChI=1S/C23H26ClNO2SSi/c1-23(2,3)29(4,5)27-20(26)15-19-21(16-11-13-18(24)14-12
InchiKey: OMLLTZCILJHLIW-UHFFFAOYSA-N
Formula: C23H26ClNO2SSi
SMILES: CC(C)(C)[Si](C)(C)OC(=O)Cc1sc(-c2ccccc2)nc1-c1ccc(Cl)cc1
Mol. weight [g/mol]: 444.06

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.11		Crippen Method
logp	7.221		Crippen Method
rinsol	3123.90		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258572&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/73-701-2/Fentiazac-TBDMS.pdf>

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