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
rinpol	3123.90		NIST Webbook
rinpol	3123.90		NIST Webbook

Sources

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=R258572&Units=SI
Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws: Log10 of Water solubility in mol/l
logp: Octanol/Water partition coefficient
rinpol: Non-polar retention indices