

Fenclofenac, TBDMS

Inchi: InChI=1S/C20H24Cl2O3Si/c1-20(2,3)26(4,5)25-18(23)13-14-9-6-7-12-17(14)24-19-15(21)
InchiKey: ZJMAOQMSSHBISI-UHFFFAOYSA-N
Formula: C20H24Cl2O3Si
SMILES: CC(C)(C)[Si](C)(C)OC(=O)Cc1cccc1Oc1c(Cl)cccc1Cl
Mol. weight [g/mol]: 411.39

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.70		Crippen Method
logp	6.877		Crippen Method
rinpol	2523.90		NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258552&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

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/38-792-1/Fenclofenac-TBDMS.pdf>

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