

Pirprofen, TBDMS

Inchi: InChI=1S/C19H28ClNO2Si/c1-14(18(22)23-24(5,6)19(2,3)4)15-9-10-17(16(20)13-15)21-
InchiKey: IRHAXCVOOJPAKQ-UHFFFAOYSA-N
Formula: C19H28ClNO2Si
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccc(N2CC=CC2)c(Cl)c1
Mol. weight [g/mol]: 365.97

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.26		Crippen Method
logp	5.368		Crippen Method
rinpol	2392.10		NIST Webbook

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=R258681&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/29-694-0/Pirprofen-TBDMS.pdf>

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