

Suprofen, TBDMS

Inchi: InChI=1S/C20H26O3SSi/c1-14(19(22)23-25(5,6)20(2,3)4)15-9-11-16(12-10-15)18(21)17
InchiKey: WLJPZTZKRFFADQ-UHFFFAOYSA-N
Formula: C20H26O3SSi
SMILES: CC(C(=O)O[Si](C)(C)C(C)(C)C)c1ccc(C(=O)c2cccs2)cc1
Mol. weight [g/mol]: 374.57

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.80		Crippen Method
logp	5.631		Crippen Method
rinpol	2621.50		NIST Webbook

Sources

Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws
NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258705&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/14-486-7/Suprofen-TBDMS.pdf>

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