

Sulindac, TBDMS

Inchi: InChI=1S/C26H31FO3SSi/c1-17-22(14-18-8-11-20(12-9-18)31(5)29)21-13-10-19(27)15-2
InchiKey: AJSZHYXITJEJDK-HMAPJEAMSA-N
Formula: C26H31FO3SSi
SMILES: CC1=C(CC(=O)O[Si](C)(C)C(C)(C)C)c2cc(F)ccc2C1=Cc1ccc(S(C)=O)cc1
Mol. weight [g/mol]: 470.67

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.30		Crippen Method
logp	6.829		Crippen Method
rinpol	3532.00		NIST Webbook
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Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258696&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/77-318-4/Sulindac-TBDMS.pdf>

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