

Diflunisal, TBDMS

Inchi: InChI=1S/C25H36F2O3Si2/c1-24(2,3)31(7,8)29-22-12-11-17(18-13-19(26)16-20(27)14-1
InchiKey: OVGKOLNSTGJEHN-UHFFFAOYSA-N
Formula: C25H36F2O3Si2
SMILES: CC(C)(C)[Si](C)(C)OC(=O)c1cc(-c2cc(F)cc(F)c2)ccc1O[Si](C)(C)C(C)(C)C
Mol. weight [g/mol]: 478.72

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.39		Crippen Method
logp	8.178		Crippen Method
rinpol	2567.90		NIST Webbook

Sources

NIST Webbook: <http://webbook.nist.gov/cgi/cbook.cgi?ID=R258547&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/72-281-0/Diflunisal-TBDMS.pdf>

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