

Niflumic acid, hydroxy, bis-methylated

Inchi:	InChI=1S/C15H13F3N2O3/c1-22-12-6-5-9(8-11(12)15(16,17)18)20-13-10(14(21)23-2)4-3
InchiKey:	RDYSEXJHOUBKCCQ-UHFFFAOYSA-N
Formula:	C15H13F3N2O3
SMILES:	COC(=O)c1cccnc1Nc1ccc(OC)c(C(F)(F)F)c1
Mol. weight [g/mol]:	326.27

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.51		Crippen Method
logp	3.639		Crippen Method
mcvol	213.270	ml/mol	McGowan Method
rinsol	2140.00		NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201813&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.cheméo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinsol:	Non-polar retention indices

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