

Niflumic acid methyl derivative

Other names:	Niflumic acid, methyl ester
Inchi:	InChI=1S/C14H11F3N2O2/c1-21-13(20)11-6-3-7-18-12(11)19-10-5-2-4-9(8-10)14(15,16)
InchiKey:	GDDOBIMJBJFCTR-UHFFFAOYSA-N
Formula:	C14H11F3N2O2
SMILES:	<chem>COC(=O)c1cccnc1Nc1cccc(C(F)(F)F)c1</chem>
Mol. weight [g/mol]:	296.24
CAS:	59361-45-4

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.39		Crippen Method
logp	3.631		Crippen Method
mcvol	193.310	ml/mol	McGowan Method
rinsol	1918.30		NIST Webbook
rinsol	1960.00		NIST Webbook

Sources

Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws
McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C59361454&Units=SI

Legend

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

Latest version available from:

<https://www.cheméo.com/cid/82-572-6/Niflumic-acid-methyl-derivative.pdf>

Generated by Cheméo on 2024-04-29 11:43:37.205197521 +0000 UTC m=+16680266.125774833.

Cheméo (<https://www.cheméo.com>) is the biggest free database of chemical and physical data for the process industry.