

Indomethacin, ethyl ester

Inchi:	InChI=1S/C21H20ClNO4/c1-4-27-20(24)12-17-13(2)23(19-10-9-16(26-3)11-18(17)19)21
InchiKey:	COIRSVPTDJIIKY-UHFFFAOYSA-N
Formula:	C21H20ClNO4
SMILES:	CCOC(=O)Cc1c(C)n(C(=O)c2ccc(Cl)cc2)c2ccc(OC)cc12
Mol. weight [g/mol]:	385.84

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.48		Crippen Method
logp	4.406		Crippen Method
mcvol	281.170	ml/mol	McGowan Method
rinpol	3038.00		NIST Webbook
rinpol	3038.00		NIST Webbook

Sources

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
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=U393583&Units=SI

Legend

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

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