Indomethacin, methyl ester

Other names:	1H-Indole-3-acetic acid, 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-, methyl ester
	Indole-3-acetic acid, 1-(p-chlorobenzoyl)-5-methoxy-2-methyl-, methyl ester
	1-(p-Chlorobenzoyl)-5-methoxy-2-methyl-3-indoleacetic acid methyl ester
	Methyl ester of indomethacin
	Indomethacine, methyl ester
	Indomethacin, methylated
	Indomethacin, methyl deriv.
	methyl 1-(4-chlorobenzoyl)-5-methoxy-2-methyl-1H-indole-3-acetate
Inchi:	InChI=1S/C20H18ClNO4/c1-12-16(11-19(23)26-3)17-10-15(25-2)8-9-18(17)22(12)20(24)
InchiKey:	OKHORWCUMZIORR-UHFFFAOYSA-N
Formula:	C20H18ClNO4
SMILES:	COC(=O)Cc1c(C)n(C(=O)c2ccc(Cl)cc2)c2ccc(OC)cc12
Mol. weight [g/mol]:	371.81
CAS:	1601-18-9

Physical Properties

Property code	Value	Unit	Source
log10ws	-6.06		Crippen Method
logp	4.016		Crippen Method
mcvol	267.080	ml/mol	McGowan Method

Sources

McGowan Method:	http://link.springer.com/article/10.1007/BF02311772
NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C1601189&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
Crippen Method:	https://www.chemeo.com/doc/models/crippen_log10ws

Legend

log10ws:	Log10 of Water solubility in mol/l

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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