

Indometacin, methylated

Other names:	Indometacin, methyl ester
Inchi:	InChI=1S/C20H19NO4/c1-13-16(12-19(22)25-3)17-11-15(24-2)9-10-18(17)21(13)20(23)
InchiKey:	WSUSASHXYDWAHF-UHFFFAOYSA-N
Formula:	C20H19NO4
SMILES:	<chem>COC(=O)Cc1c(C)n(C(=O)c2ccccc2)c2ccc(OC)cc12</chem>
Mol. weight [g/mol]:	337.37

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.37		Crippen Method
logp	3.362		Crippen Method
mcvol	254.840	ml/mol	McGowan Method

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=R201680&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci9903071
Crippen Method:	https://www.chemeo.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

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<https://www.chemeo.com/cid/98-175-0/Indometacin-methylated.pdf>

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