Indomethacin, pentyl ester

Inchi: InChI=1S/C24H26ClNO4/c1-4-5-6-13-30-23(27)15-20-16(2)26(22-12-11-19(29-3)14-21(2
InchiKey: QTYWTQHCPSOERT-UHFFFAOYSA-N
Formula: C24H26ClNO4
SMILES: CCCCCOC(=O)Cc1c(C)n(C(=O)c2ccc(Cl)cc2)c2ccc(OC)cc12
Mol. weight [g/mol]: 427.92

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.73		Crippen Method
logp	5.576		Crippen Method
mcvol	323.440	ml/mol	McGowan Method
rinpol	3304.00		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=U394019&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