

Indomethacin, isobutyl ester

Inchi: InChI=1S/C23H24ClNO4/c1-14(2)13-29-22(26)12-19-15(3)25(21-10-9-18(28-4)11-20(19)
InchiKey: MBMGSPXVGDYMEF-UHFFFAOYSA-N
Formula: C₂₃H₂₄ClNO₄
SMILES: COc1ccc2c(c1)c(CC(=O)OCC(C)C)c(C)n2C(=O)c1ccc(Cl)cc1
Mol. weight [g/mol]: 413.89

Physical Properties

Property code	Value	Unit	Source
log10ws	-7.07		Crippen Method
logp	5.042		Crippen Method
mcvol	309.350	ml/mol	McGowan Method
rinpole	3159.00		NIST Webbook
rinpole	3159.00		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=U393969&Units=SI>

Legend

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

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