

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: QTYWTQHCPISOERT-UHFFFAOYSA-N
Formula: C₂₄H₂₆ClNO₄
SMILES: CCCCCOC(=O)C1c(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/ci9903071>
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

Latest version available from:

<https://www.chemeo.com/cid/77-414-7/Indomethacin-pentyl-ester.pdf>

Generated by Cheméo on 2024-04-28 00:48:49.958868012 +0000 UTC m=+16554578.879445406.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.