

Indometacin, hydroxy, bis-methylated

Other names: Hydroxyindomethacin, bis-methylated
Inchi: InChI=1S/C21H21NO5/c1-13-17(12-20(23)27-4)18-11-16(26-3)9-10-19(18)22(13)21(24)
InchiKey: RKLGIVJTSFHOH-UHFFFAOYSA-N
Formula: C₂₁H₂₁NO₅
SMILES: COC(=O)Cc1c(C)n(C(=O)c2ccc(OC)cc2)c2ccc(OC)cc12
Mol. weight [g/mol]: 367.40

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.49		Crippen Method
logp	3.371		Crippen Method
mcvol	274.800	ml/mol	McGowan Method
rinpol	2880.00		NIST Webbook
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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=R201655&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

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