Etodolac, methylated

Inchi: InChI=1S/C18H23NO3/c1-4-12-7-6-8-13-14-9-10-22-18(5-2,11-15(20)21-3)17(14)19-16(1
InchiKey: CRRWJZHQYUTACF-UHFFFAOYSA-N
Formula: C18H23NO3
SMILES: CCc1cccc2c3c([nH]c12)C(CC)(CC(=O)OC)OCC3
Mol. weight [g/mol]: 301.38

Physical Properties

Property code	Value	Unit	Source
log10ws	-4.59		Crippen Method
logp	2.989		Crippen Method
mcvol	237.990	ml/mol	McGowan Method
rinpol	2225.00		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=R201571&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