Dimetindene M (nor, OH), acetylated

Inchi: InChI=1S/C23H26N2O3/c1-15(22-7-5-6-11-24-22)23-18(10-12-25(4)16(2)26)13-19-14-20
InchiKey: CPMRHZBAZYTLGT-UHFFFAOYSA-N
Formula: C23H26N2O3
SMILES: CC(=O)Oc1ccc2c(c1)CC(CCN(C)C(C)=O)=C2C(C)c1ccccn1
Mol. weight [g/mol]: 378.46

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.51		Crippen Method
logp	3.989		Crippen Method
mcvol	301.220	ml/mol	McGowan Method
rinpol	3090.00		NIST Webbook
rinpol	3090.00		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=R120635&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

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