

Dimetindene M (nor), acetylated

Inchi: InChI=1S/C21H24N2O/c1-15(20-10-6-7-12-22-20)21-18(11-13-23(3)16(2)24)14-17-8-4-5
InchiKey: NRYFWAGHSWKXMA-UHFFFAOYSA-N
Formula: C21H24N2O
SMILES: CC(=O)N(C)CCC1=C(C(C)c2ccccc2)c2ccccc2C1
Mol. weight [g/mol]: 320.43

Physical Properties

Property code	Value	Unit	Source
log10ws	-5.19		Crippen Method
logp	4.063		Crippen Method
mcvol	265.600	ml/mol	McGowan Method
rinpol	2775.00		NIST Webbook
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Sources

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=R120620&Units=SI>
Crippen Method: <http://pubs.acs.org/doi/abs/10.1021/ci990307l>

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/10-639-1/Dimetindene-M-nor-acetylated.pdf>

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