

Tolmetin

Other names:

1-Methyl-5-(4-methylbenzoyl)-pyrrole-2-acetic acid
1-Methyl-5-p-toluoyl-pyrrole-2-acetic acid
1H-Pyrrole-2-acetic acid, 1-methyl-5-(4-methylbenzoyl)-
Acido 1-metil-5-(p-tolnil)-pirrol-2-acetico
McN 2559
Pyrrole-2-acetic acid, 1-methyl-5-p-toluoyl-
Tolmetine

Inchi: InChI=1S/C15H15NO3/c1-10-3-5-11(6-4-10)15(19)13-8-7-12(16(13)2)9-14(17)18/h3-8H,**InchiKey:** UPSPUYADGBWSHF-UHFFFAOYSA-N**Formula:** C15H15NO3**SMILES:** Cc1ccc(C(=O)c2ccc(CC(=O)O)n2C)cc1**Mol. weight [g/mol]:** 257.28**CAS:** 26171-23-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.96		Aqueous Solubility Prediction Method
logp	2.192		Crippen Method
mccvol	197.980	ml/mol	McGowan Method

Sources

Aqueous Solubility Prediction Method: <http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx>**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C26171233&Units=SI>**Crippen Method:** <http://pubs.acs.org/doi/abs/10.1021/ci9903071>

Legend

log10ws: Log10 of Water solubility in mol/l**logp:** Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume

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