1H-Pyrrole-2-acetic acid, 1-methyl-5-(4-methylbenzoyl)-

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

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]: 257.29

Physical Properties

Property code	Value	Unit	Source
hf	-406.57	kJ/mol	Cheméo Relay (1.0)
ie	8.04	eV	Cheméo Relay (1.0)
log10ws	-2.96		Aqueous Solubility Prediction Method
logp	2.192		Crippen Method
mcvol	197.980	ml/mol	McGowan Method
tb	640.30	K	Cheméo Relay (1.0)
tc	930.62	K	Cheméo Relay (1.0)
tf	440.75	K	Cheméo Relay (1.0)

Sources

Crippen Method: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

Aqueous Solubility Prediction Method: http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C26171233&Units=SI

McGowan Method: http://link.springer.com/article/10.1007/BF02311772

Legend

hf:	Enthalpy of formation at standard conditions
ie:	Ionization energy
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point