4-CHLORO-3-(3-METHYL-5-OXO-2-PYRAZOLIN-1-ACID

Other names: Benzenesulfonic acid, 4-chloro-3-(4,5-dihydro-3-methyl-5-oxo-1H-pyrazol-1-yl)-
Benzenesulfonic acid, 4-chloro-3-(3-methyl-5-oxo-2-pyrazolin-1-yl)-
4-Chloro-3-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulfonic acid
4-chloro-3-(3-methyl-5-oxo-2-pyrazolin-1-yl)benzenesulphonic acid

Inchi: InChI=1S/C10H9ClN2O4S/c1-6-4-10(14)13(12-6)9-5-7(18(15,16)17)2-3-8(9)11/h2-3,5H,4

InchiKey: UWLNKHDLVZEYKQ-UHFFFAOYSA-N

Formula: C10H9ClN2O4S

SMILES: CC1=NN(c2cc(S(=O)(=O)O)ccc2Cl)C(=O)C1

Mol. weight [g/mol]: 288.71

Physical Properties

Property code	Value	Unit	Source
ie	8.74	eV	Cheméo Relay (1.0)
logp	1.699		Crippen Method
mcvol	180.570	ml/mol	McGowan Method

Sources

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

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

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Cheméo Relay (1.0):

Cheméo Relay (1.0, beta):

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C88766&Units=SI

Legend

ie: Ionization energy

logp: Octanol/Water partition coefficient

mcvol: McGowan's characteristic volume