

1-(2'-Chloro-5'-sulfophenyl)-3-methyl-5-pyrazolone

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:	<chem>CC1=NN(c2cc(S(=O)(=O)O)ccc2Cl)C(=O)C1</chem>
Mol. weight [g/mol]:	288.71
CAS:	88-76-6

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.32		Crippen Method
logp	1.699		Crippen Method
mcvol	180.570	ml/mol	McGowan Method

Sources

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

Legend

log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume

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