1-(3-Chlorophenyl)-3-methyl-2-pyrazolin-5-one

Other names:	m-Chloropyrazone
	1-(m-Chlorophenyl)-3-methyl-5-pyrazolone
	1-(3-Chlorophenyl)-3-methyl-5-pyrazolone
	(m-Chlorophenyl)-3-methyl-2-pyrazolin-5-one
Inchi:	InChI=1S/C10H9ClN2O/c1-7-5-10(14)13(12-7)9-4-2-3-8(11)6-9/h2-4,6H,5H2,1H3
InchiKey:	RIOMUJXIGYZENC-UHFFFAOYSA-N
Formula:	C10H9ClN2O
SMILES:	CC1=NN(c2cccc(Cl)c2)C(=O)C1
Mol. weight [g/mol]:	208.64
CAS:	20629-90-7

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.73		Crippen Method
logp	2.453		Crippen Method
mcvol	146.610	ml/mol	McGowan Method

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=C20629907&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