4,5-Isoxazoledione, 3-methyl-, 4-[(2-chlorophenyl)hydrazone]

Other names: 4,5-Isoxazoledione, 3-methyl-, 4-[(2-chlorophenyl)hydrazone]
4,5-Isoxazoledione, 3-methyl-, 4-[(o-chlorophenyl)hydrazone]
JF 1633
JF 2067
Mil-Col (pesticide)
Milcol
PP 781
R 22395
4-(2-Chlorophenylhydrazone)-3-methyl-5-isoxazolone
4-(2-Chlorophenylhydrazono)-3-methyl-5(4H)-isoxazolone
Drazoxolone
Ganocide
3-Methyl-4-((o-chlorophenyl)hydrazone)-4,5-isoxazoledione
3-Methyl-4-(o-chlorophenylhydrazono)-5-isoxazolone
3-Methyl-4,5-isoxazoledione 4-((2-chlorophenyl)hydrazone)
Saisan
Sopracol
Sopracol 781
3-Methyl-4-[(2-chlorophenyl)hydrazone]-4,5-isoxazoledione
Drazoxolan

Inchi: InChI=1S/C10H8ClN3O2/c1-6-9(10(15)16-14-6)13-12-8-5-3-2-4-7(8)11/h2-5,12H,1H3

InchiKey: OOTHTARUZHONSW-UHFFFAOYSA-N

Formula: C10H8ClN3O2

SMILES: CC1=NOC(=O)C1=NNc1ccccc1Cl

Mol. weight [g/mol]: 237.65

Physical Properties

Property code	Value	Unit	Source
logp	2.041		Crippen Method
mcvol	158.160	ml/mol	McGowan Method
tf	441.18 ± 0.20	K	NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	28.04	kJ/mol	440.40	NIST Webbook

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=C5707697&Units=SI
Joback Method: https://en.wikipedia.org/wiki/Joback_method

Legend

hfust: Enthalpy of fusion at a given temperature
logp: Octanol/Water partition coefficient
mcvol: McGowan's characteristic volume
tf: Normal melting (fusion) point