

# Oxadiazon

## Other names:

1,3,4-Oxadiazol-2(3H)-one,  
 3-[2,4-dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-  
 1,3,4-Oxadiazol-2(3H)-one,  
 3-(2,4-dichloro-5-(1-methylethoxy)phenyl)-5-(1,1-dimethylethyl)-  
 17623 RP  
 2-tert-Butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-1,3,4-oxadiazolin-5-one  
 3-(2,4-Dichloro-5-isopropoxy-phenyl)-«delta»4-5-(tert-butyl)-1,3,4-oxadiazoline-2-one  
 3-(2,4-Dichloro-5-isopropoxy-phenyl)-Â«deltaÂ»4-5-(tert-butyl)-1,3,4-oxadiazoline-2-one  
 3-[2,4-Dichloro-5-(1-methylethoxy)phenyl]-5-(1,1-dimethylethyl)-1,3,4-oxadiazol-2(3H)-on  
 5-tert-butyl-3-(2,4-dichloro-5-propan-2-yloxyphenyl)-1,3,4-oxadiazol-2-one  
 G 315  
 Oxadiazone  
 Oxydiazon  
 RP 17,623  
 RP 17623  
 Ronstar  
 Ronstar 50W  
 Scotts OH I

## Inchi:

«DELTA»2-1,3,4-Oxadiazolin-5-one,  
 2-tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-  
 «DELTA»2-1,3,4-Oxadiazolin-5-one,  
 2-tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-  
 A«DELTA»2-1,3,4-Oxadiazolin-5-one,  
 2-tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-  
 A«DELTA»2-1,3,4-Oxadiazolin-5-one,  
 2-tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-  
 mChI=1S/C15H18Cl2N2O3/c1-8(2)21-12-17-11(9(16)6-10(12)17)19-14(20)22-13(18-19)1

## InchiKey:

CHNUNORXWHYHNE-UHFFFAOYSA-N

## Formula:

C15H18Cl2N2O3

## SMILES:

CC(C)Oc1cc(-n2nc(C(C)(C)C)oc2=O)c(Cl)cc1Cl

## Mol. weight [g/mol]:

345.22

## CAS:

19666-30-9

## Physical Properties

Property code	Value	Unit	Source
log10ws	-5.69		Aqueous Solubility Prediction Method
log10ws	-5.70		Estimated Solubility Method
logp	4.217		Crippen Method
mcvol	241.040	ml/mol	McGowan Method
rinpol	2189.00		NIST Webbook
rinpol	2159.00		NIST Webbook

rinpol	2200.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2186.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2198.00		NIST Webbook
rinpol	2189.00		NIST Webbook
rinpol	2187.00		NIST Webbook
rinpol	2182.00		NIST Webbook
rinpol	2138.00		NIST Webbook
rinpol	2182.00		NIST Webbook
ripol	2948.00		NIST Webbook
tf	361.25 ± 0.20	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	26.39	kJ/mol	360.60	NIST Webbook

## Sources

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Aqueous Solubility Prediction Method:**

<http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa>

**Estimated Solubility Method:**

[http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl\\_file/ci034243xsi20040112\\_053635.txt](http://pubs.acs.org/doi/suppl/10.1021/ci034243x/suppl_file/ci034243xsi20040112_053635.txt)

**McGowan Method:**

<http://link.springer.com/article/10.1007/BF02311772>

**NIST Webbook:**

<http://webbook.nist.gov/cgi/cbook.cgi?ID=C19666309&Units=SI>

## Legend

<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>log10ws:</b>	Log10 of Water solubility in mol/l
<b>logp:</b>	Octanol/Water partition coefficient
<b>mcvol:</b>	McGowan's characteristic volume
<b>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices

**tf:** Normal melting (fusion) point

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