Triadimefon

Other names: 1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)-butan-2-one
1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-2-butanone
1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)butan-2-one
1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)butanone
1-(4-chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl) butan-2-one
1H-1,2,4-Triazole, 1-((tert-butylcarbonyl-4-chlorophenoxy)methyl)-
2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1,2,4-triazol-1-yl)-
2-Butanone, 1-(4-chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)-
Amiral
Azocene
BAY 6681F
BAY-MEB 6447
Bayleton
Bayleton 250 EC
Bayleton 5
Bayleton special
MEB 6447
NSC 303303
Reach
Tartan (fungicide)
Tidifon
Triadimefone
Tridimefon
bayletone
chlorophenoxy)butanone
{1-(4-Chlorophenoxy)-3,3-dimethyl-1-(1H-1,2,4-triazol-1-yl)}butanone (triadimefon)

Inchi: InChI=1S/C14H16ClN3O2/c1-14(2,3)12(19)13(18-9-16-8-17-18)20-11-6-4-10(15)5-7-11/h

InchiKey: WURBVZBTWMNKQT-UHFFFAOYSA-N

Formula: C14H16ClN3O2

SMILES: CC(C)(C)C(=O)C(Oc1ccc(Cl)cc1)n1cncn1

Mol. weight [g/mol]: 293.75

CAS: 43121-43-3

Physical Properties

Property code	Value	Unit	Source
log10ws	-3.61		Estimated Solubility Method

log10ws	-3.61		Aqueous Solubility Prediction Method
logp	3.124		Crippen Method
mcvol	214.520	ml/mol	McGowan Method
rinpol	1939.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1968.00		NIST Webbook
rinpol	1990.00		NIST Webbook
rinpol	1999.00		NIST Webbook
rinpol	1997.00		NIST Webbook
rinpol	1966.00		NIST Webbook
rinpol	1981.00		NIST Webbook
ripol	2942.00		NIST Webbook
tf	350.20 ± 0.50	K	NIST Webbook
tf	353.62 ± 0.20	K	NIST Webbook
tf	355.45	K	Aqueous Solubility Prediction Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	22.87	kJ/mol	351.40	NIST Webbook
hsubt	111.10 ± 2.20	kJ/mol	320.50	NIST Webbook

Sources

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

Solubilities of Triadimefon in Acetone + Water from (278.15 to 333.15) K: https://www.doi.org/10.1021/je900045z

Solubility of Triadimefon in Organic Solvents at Temperatures between (288.15 and 333.15) K: https://www.doi.org/10.1021/je901024t

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

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

NIST Webbook: http://webbook.nist.gov/cgi/cbook.cgi?ID=C43121433&Units=SI

Legend

hfust:	Enthalpy of fusion at a given temperature
hsubt:	Enthalpy of sublimation at a given temperature
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
rinpol:	Non-polar retention indices
ripol:	Polar retention indices
tf:	Normal melting (fusion) point