Terbacil

Other names:	2,4(1H,3H)-Pyrimidinedione, 5-chloro-3-(1,1-dimethylethyl)-6-methyl-
	3-tert-Butyl-5-Chloro-6-methyluracil
	3-tert-butyl-5-chloro-6-methyl-1H-pyrimidine-2,4-dione
	3-tert.Butyl-5-chlor-6-methyluracil
	5-Chloro-3-(1,1-dimethylethyl)-6-methyl-2,4(1H,3H)-pyrimidinedione
	5-Chloro-3-(1,1-dimethylethyl)-6-methyl-pyrimidinedione
	5-Chloro-3-tert-butyl-6-methyluracil
	Compound 732
	DPX-D732
	Du Pont 732
	Du Pont herbicide 732
	Experimental Herbicide 732
	Geonter
	Herbicide 732
	Sinbar
	Turbacil
	Uracil, 3-tert-butyl-5-chloro-6-methyl-
Inchi:	InChI=1S/C9H13ClN2O2/c1-5-6(10)7(13)12(8(14)11-5)9(2,3)4/h1-4H3,(H,11,14)
InchiKey:	NBQCNZYJJMBDKY-UHFFFAOYSA-N
Formula:	C8H13ClN2O2
SMILES:	Cc1[nH]c(=O)n(C(C)(C)C)c(=O)c1Cl
Mol. weight [g/mol]:	204.65
CAS:	5902-51-2

Physical Properties

Property code	Value	Unit	Source
log10ws	-2.48		Aqueous Solubility Prediction Method
log10ws	-2.48		Estimated Solubility Method
logp	0.772		Crippen Method
mcvol	157.850	ml/mol	McGowan Method
rinpol	1816.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1800.00		NIST Webbook
rinpol	1836.00		NIST Webbook

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	12.51	kJ/mol	448.00	NIST Webbook

Sources

NIST Webbook:	http://webbook.nist.gov/cgi/cbook.cgi?ID=C5902512&Units=SI
Crippen Method:	http://pubs.acs.org/doi/abs/10.1021/ci990307l
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

Legend

hfust:	Enthalpy of fusion 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

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