

# Isocil

<b>Other names:</b>	2,4(1H,3H)-Pyrimidinedione, 5-bromo-6-methyl-3-(1-methylethyl)- Uracil, 5-bromo-3-isopropyl-6-methyl- H-82 Hyvar 5-Bromo-6-Methyl-3-(1-methylethyl)-2,4(1H,3H)-pyrimidinedione Herbicide 82 Isoprocil KC 1215 3-Isopropyl-5-bromo-6-methyluracil 5-Brom-3-isopropyl-6-methyl-uracil 5-Bromo-3-isopropyl-6-methyl, 2,4-pyrimidinedione 5-Bromo-3-isopropyl-6-methyluracil 5-Bromo-3-isopropyl-6-metil-uracil 5-Broom-3-isopropyl-6-methyl-uracil- 5-Broom-3-isopropyl-6-methyl-uracil-(Dutch) Du Pont herbicide 82 NSC 75241
<b>Inchi:</b>	InChI=1S/C8H11BrN2O2/c1-4(2)11-7(12)6(9)5(3)10-8(11)13/h4H,1-3H3,(H,10,13)
<b>InchiKey:</b>	PSYBGEADHLUXCS-UHFFFAOYSA-N
<b>Formula:</b>	C8H11BrN2O2
<b>SMILES:</b>	Cc1[nH]c(=O)n(C(C)C)c(=O)c1Br
<b>Mol. weight [g/mol]:</b>	247.09
<b>CAS:</b>	314-42-1

## Physical Properties

Property code	Value	Unit	Source
log10ws	-1.82		Crippen Method
logp	0.707		Crippen Method
mcvol	149.020	ml/mol	McGowan Method

## Sources

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

**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C314421&Units=SI>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci990307l>

**Crippen Method:**

[https://www.cheméo.com/doc/models/crippen\\_log10ws](https://www.cheméo.com/doc/models/crippen_log10ws)

## Legend

**log10ws:** Log10 of Water solubility in mol/l  
**logp:** Octanol/Water partition coefficient  
**mcvol:** McGowan's characteristic volume

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