

# Ipazine

**Other names:**

1,3,5-Triazine-2,4-diamine, 6-chloro-N,N-diethyl-N'-(1-methylethyl)-  
2-Chloro-4-(diethylamino)-6-(isopropylamino)-s-triazine  
6-chloro-N,N-diethyl-N'-propan-2-yl-1,3,5-triazine-2,4-diamine  
G 30031  
Geigy  
Gesabal  
Heptazine  
Isodiazine  
NSC 163047

**Inchi:** InChI=1S/C10H18ClN5/c1-5-16(6-2)10-14-8(11)13-9(15-10)12-7(3)4/h7H,5-6H2,1-4H3,(**InchiKey:** OWYWGLHRNBIFJP-UHFFFAOYSA-N**Formula:** C10H18ClN5**SMILES:** CCN(CC)c1nc(Cl)nc(NC(C)C)n1**Mol. weight [g/mol]:** 243.74**CAS:** 1912-25-0

## Physical Properties

Property code	Value	Unit	Source
log10ws	-3.79		Aqueous Solubility Prediction Method
log10ws	-3.79		Estimated Solubility Method
logp	2.192		Crippen Method
mcvol	190.140	ml/mol	McGowan Method
ripol	1763.00		NIST Webbook
ripol	1763.00		NIST Webbook
ripol	2461.00		NIST Webbook
ripol	2475.00		NIST Webbook
ripol	2461.00		NIST Webbook

## Sources

**McGowan Method:** <http://link.springer.com/article/10.1007/BF02311772>**NIST Webbook:** <http://webbook.nist.gov/cgi/cbook.cgi?ID=C1912250&Units=SI>

**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)

## Legend

<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

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