

# Isoproturon

<b>Other names:</b>	1,1-dimethyl-3-(4-propan-2-ylphenyl)urea 3-(4-Isopropylphenyl)-1,1-dimethylurea Alon Arelon Arelon R Belgran CGA-18731 CL 12150 DPX 6774 Graminon HOE 16410 Hytane 500L IP 50 IP-Flo IPU Stefes N'-(4-Isopropylphenyl)-N,N-dimethylurea N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]urea N-(4-Isopropylphenyl)-N',N'-dimethylharnstoff N-(4-Isopropylphenyl)-N',N'-dimethylurea N-4-Isopropylphenyl-N,N-dimethylurea Nocilon Protugan Tolkan Tolken Urea, 1,1-dimethyl-3-(p-isopropylphenyl)- Urea, 3-p-cumenyl-1,1-dimethyl- Urea, N,N-dimethyl-N'-[4-(1-methylethyl)phenyl]-
<b>Inchi:</b>	InChI=1S/C12H18N2O/c1-9(2)10-5-7-11(8-6-10)13-12(15)14(3)4/h5-9H,1-4H3,(H,13,15)
<b>InchiKey:</b>	PUIYMUZLKQOUOZ-UHFFFAOYSA-N
<b>Formula:</b>	C12H18N2O
<b>SMILES:</b>	CC(C)c1ccc(NC(=O)N(C)C)cc1
<b>Mol. weight [g/mol]:</b>	206.28
<b>CAS:</b>	34123-59-6

## Physical Properties

Property code	Value	Unit	Source
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gf	221.75	kJ/mol	Joback Method
hf	-62.81	kJ/mol	Joback Method
hfus	26.68	kJ/mol	Joback Method
hvap	60.08	kJ/mol	Joback Method
log10ws	-3.52	Aqueous Solubility Prediction Method	
log10ws	-3.54	Estimated Solubility Method	
logp	2.904	Crippen Method	
mcvol	177.710	ml/mol	McGowan Method
pc	2571.50	kPa	Joback Method
tb	621.66	K	Joback Method
tc	832.03	K	Joback Method
tf	430.81 ± 0.20	K	NIST Webbook
vc	0.652	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	514.38	J/mol×K	761.90	Joback Method
cpg	526.39	J/mol×K	796.97	Joback Method
cpg	457.31	J/mol×K	621.66	Joback Method
cpg	473.02	J/mol×K	656.72	Joback Method
cpg	487.74	J/mol×K	691.78	Joback Method
cpg	501.51	J/mol×K	726.84	Joback Method
cpg	537.59	J/mol×K	832.03	Joback Method
hfust	21.33	kJ/mol	427.40	NIST Webbook
hfust	33.87	kJ/mol	430.40	NIST Webbook

## Sources

<b>McGowan Method:</b>	<a href="http://link.springer.com/article/10.1007/BF02311772">http://link.springer.com/article/10.1007/BF02311772</a>
<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C34123596&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C34123596&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</a>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</a>
<b>Aqueous Solubility Prediction Method:</b>	<a href="http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDataset002.xlsx</a>
<b>Estimated Solubility Method:</b>	<a href="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</a>

# Legend

<b>cpg:</b>	Ideal gas heat capacity
<b>gf:</b>	Standard Gibbs free energy of formation
<b>hf:</b>	Enthalpy of formation at standard conditions
<b>hfus:</b>	Enthalpy of fusion at standard conditions
<b>hfust:</b>	Enthalpy of fusion at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<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>pc:</b>	Critical Pressure
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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