

# Monolinuron

<b>Other names:</b>	1-Methoxy-1-methyl-3-(4-chlorophenyl)urea 3-(4-Chlorophenyl)-1-methoxy-1-methylurea 3-(4-Chlorophenyl)-1-methoxy-1-methylharnstoff Afesin Aresin Arezin Arezine Arresin HOE 2747 Monorotox N'-(4-Chlorophenyl)-N-methoxy-N-methylurea N-(4-Chlorophenyl)-N'-methoxy-N-methylurea Premalin Urea, 3-(p-chlorophenyl)-1-methoxy-1-methyl- Urea, N'-(4-chlorophenyl)-N-methoxy-N-methyl-
<b>Inchi:</b>	InChI=1S/C9H11CIN2O2/c1-12(14-2)9(13)11-8-5-3-7(10)4-6-8/h3-6H,1-2H3,(H,11,13)
<b>InchiKey:</b>	LKJPSUCKSLORMF-UHFFFAOYSA-N
<b>Formula:</b>	C9H11CIN2O2
<b>SMILES:</b>	CON(C)C(=O)Nc1ccc(Cl)cc1
<b>Mol. weight [g/mol]:</b>	214.65
<b>CAS:</b>	1746-81-2

## Physical Properties

Property code	Value	Unit	Source
gf	82.00	kJ/mol	Joback Method
hf	-143.57	kJ/mol	Joback Method
hfus	27.82	kJ/mol	Joback Method
hvap	60.59	kJ/mol	Joback Method
log10ws	-2.57		Aqueous Solubility Prediction Method
log10ws	-2.57		Estimated Solubility Method
logp	2.365		Crippen Method
mcvol	153.550	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	613.31	K	Joback Method
tc	831.34	K	Joback Method

tf	$353.91 \pm 0.20$	K	NIST Webbook
tf	354.65	K	Aqueous Solubility Prediction Method
vc	0.557	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	414.14	J/mol×K	795.01	Joback Method
cpg	361.17	J/mol×K	613.31	Joback Method
cpg	373.34	J/mol×K	649.65	Joback Method
cpg	384.69	J/mol×K	685.99	Joback Method
cpg	395.26	J/mol×K	722.33	Joback Method
cpg	405.06	J/mol×K	758.67	Joback Method
cpg	422.50	J/mol×K	831.34	Joback Method
hfust	22.54	kJ/mol	353.40	NIST Webbook

# Sources

<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>
<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=C1746812&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1746812&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>

# 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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