

# Metolcarb

<b>Inchi:</b>	InChI=1S/C8H9NO2/c1-9-8(10)11-7-5-3-2-4-6-7/h2-6H,1H3,(H,9,10)
<b>InchiKey:</b>	SCWKRWCUMCMVPW-UHFFFAOYSA-N
<b>Formula:</b>	C8H9NO2
<b>SMILES:</b>	CNC(=O)Oc1ccccc1
<b>Mol. weight [g/mol]:</b>	151.17

## Physical Properties

Property code	Value	Unit	Source
gf	-15.64	kJ/mol	Joback Method
hf	-163.25	kJ/mol	Joback Method
hfus	18.40	kJ/mol	Joback Method
hvap	51.27	kJ/mol	Joback Method
log10ws	-1.80		Estimated Solubility Method
log10ws	-1.80		Aqueous Solubility Prediction Method
logp	1.405		Crippen Method
mvol	117.240	ml/mol	McGowan Method
pc	3925.85	kPa	Joback Method
tb	535.58	K	Joback Method
tc	755.73	K	Joback Method
tf	331.16	K	Joback Method
vc	0.434	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.09	J/mol×K	535.58	Joback Method
cpg	268.87	J/mol×K	572.27	Joback Method
cpg	279.94	J/mol×K	608.96	Joback Method
cpg	290.31	J/mol×K	645.65	Joback Method
cpg	300.01	J/mol×K	682.34	Joback Method
cpg	309.03	J/mol×K	719.03	Joback Method
cpg	317.41	J/mol×K	755.73	Joback Method

# 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/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</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>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>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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