

# Glyoxime, methylphenyl-

<b>Inchi:</b>	InChI=1S/C9H10N2O2/c1-7(10-12)9(11-13)8-5-3-2-4-6-8/h2-6,12-13H,1H3/b10-7-,11-9+
<b>InchiKey:</b>	OHOFOAMRUFMQPH-PWMCPNNSA-N
<b>Formula:</b>	C9H10N2O2
<b>SMILES:</b>	CC(=NO)C(=NO)c1ccccc1
<b>Mol. weight [g/mol]:</b>	178.19
<b>CAS:</b>	4937-86-4

## Physical Properties

Property code	Value	Unit	Source
hf	-152.16	kJ/mol	Joback Method
hvap	78.05	kJ/mol	Joback Method
log10ws	-2.30		Aqueous Solubility Prediction Method
logp	1.715		Crippen Method
mcvol	137.010	ml/mol	McGowan Method
pc	3202.78	kPa	Joback Method
tb	769.48	K	Joback Method
tc	985.86	K	Joback Method

## 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=C4937864&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4937864&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/AqueousDa">http://onschallenge.wikispaces.com/file/view/AqueousDataset002.xlsx/351826032/AqueousDa</a>

## Legend

<b>hf:</b>	Enthalpy of formation 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

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