

# 4-Methoxyisonitrosoacetanilide

<b>Inchi:</b>	InChI=1S/C9H10N2O3/c1-14-8-4-2-7(3-5-8)11-9(12)6-10-13/h2-6,13H,1H3,(H,11,12)/b1
<b>InchiKey:</b>	MDEHFNBKDPLEEJ-UXBLZVDNSA-N
<b>Formula:</b>	C9H10N2O3
<b>SMILES:</b>	COc1ccc(NC(=O)C=NO)cc1
<b>Mol. weight [g/mol]:</b>	194.19
<b>CAS:</b>	6335-41-7

## Physical Properties

Property code	Value	Unit	Source
hf	-265.37	kJ/mol	Joback Method
hvap	74.15	kJ/mol	Joback Method
log10ws	-0.61		Crippen Method
logp	1.094		Crippen Method
mcvol	142.880	ml/mol	McGowan Method
pc	3380.21	kPa	Joback Method
tb	732.30	K	Joback Method
tc	947.81	K	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	8.30	kJ/mol	457.60	NIST Webbook
hfust	8.30	kJ/mol	459.00	NIST Webbook
sfust	18.10	J/molxK	459.00	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=C6335417&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6335417&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>Crippen Method:</b>	<a href="https://www.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</a>

## Legend

<b>hf:</b>	Enthalpy of formation 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>sfust:</b>	Entropy of fusion at a given temperature
<b>tb:</b>	Normal Boiling Point Temperature
<b>tc:</b>	Critical Temperature

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