

# 2-Chloroisnitrosoacetanilide

<b>Inchi:</b>	InChI=1S/C8H7ClN2O2/c9-6-3-1-2-4-7(6)11-8(12)5-10-13/h1-5,13H,(H,11,12)/b10-5+
<b>InchiKey:</b>	VFTUFVGOXLZZPW-BJMVGYQFSA-N
<b>Formula:</b>	C8H7ClN2O2
<b>SMILES:</b>	O=C(C=NO)Nc1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	198.61
<b>CAS:</b>	14722-82-8

## Physical Properties

Property code	Value	Unit	Source
hf	-128.25	kJ/mol	Joback Method
hvac	73.90	kJ/mol	Joback Method
log10ws	-1.18		Crippen Method
logp	1.738		Crippen Method
mccvol	135.160	ml/mol	McGowan Method
pc	3699.95	kPa	Joback Method
tb	724.43	K	Joback Method
tc	948.67	K	Joback Method
tf	429.00 ± 1.00	K	NIST Webbook

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
hfust	29.70	kJ/mol	432.70	NIST Webbook
hfust	29.70	kJ/mol	429.00	NIST Webbook
sfust	69.30	J/mol×K	429.00	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>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=C14722828&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C14722828&amp;Units=SI</a>

**Crippen Method:**

<http://pubs.acs.org/doi/abs/10.1021/ci9903071>

**Crippen Method:**

[https://www.chemeo.com/doc/models/crippen\\_log10ws](https://www.chemeo.com/doc/models/crippen_log10ws)

## 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
<b>tf:</b>	Normal melting (fusion) point

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