

# M-chlorocarbanilic acid, 2-cyanoethyl ester

<b>Inchi:</b>	InChI=1S/C10H9CIN2O2/c11-8-3-1-4-9(7-8)13-10(14)15-6-2-5-12/h1,3-4,7H,2,6H2,(H,13
<b>InchiKey:</b>	MPBQWHXSXRKKPK-UHFFFAOYSA-N
<b>Formula:</b>	C10H9CIN2O2
<b>SMILES:</b>	N#CCCOC(=O)Nc1cccc(Cl)c1
<b>Mol. weight [g/mol]:</b>	224.64
<b>CAS:</b>	5330-47-2

## Physical Properties

Property code	Value	Unit	Source
gf	112.82	kJ/mol	Joback Method
hf	-66.86	kJ/mol	Joback Method
hfus	28.90	kJ/mol	Joback Method
hvap	71.25	kJ/mol	Joback Method
log10ws	-3.13		Crippen Method
logp	2.802		Crippen Method
mvol	159.040	ml/mol	McGowan Method
pc	2875.03	kPa	Joback Method
tb	725.83	K	Joback Method
tc	955.38	K	Joback Method
tf	461.13	K	Joback Method
vc	0.622	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	389.52	J/molxK	725.83	Joback Method
cpg	399.20	J/molxK	764.09	Joback Method
cpg	408.13	J/molxK	802.35	Joback Method
cpg	416.31	J/molxK	840.60	Joback Method
cpg	423.77	J/molxK	878.86	Joback Method
cpg	430.52	J/molxK	917.12	Joback Method
cpg	436.59	J/molxK	955.38	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>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=C5330472&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C5330472&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307l">http://pubs.acs.org/doi/abs/10.1021/ci990307l</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>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

Latest version available from:

<https://www.chemeo.com/cid/48-849-7/M-chlorocarbanilic-acid-2-cyanoethyl-ester.pdf>

Generated by Cheméo on 2024-04-29 09:32:17.979284752 +0000 UTC m=+16672386.899862067.

Cheméo (<https://www.chemeo.com>) is the biggest free database of chemical and physical data for the process industry.