

# 2-Chloro-n,n-bis(2-cyanoethyl)benzamide

<b>Inchi:</b>	InChI=1S/C13H12ClN3O/c14-12-6-2-1-5-11(12)13(18)17(9-3-7-15)10-4-8-16/h1-2,5-6H,3
<b>InchiKey:</b>	RAJQRBVEXOUFAX-UHFFFAOYSA-N
<b>Formula:</b>	C13H12ClN3O
<b>SMILES:</b>	N#CCCN(CCC#N)C(=O)c1ccccc1Cl
<b>Mol. weight [g/mol]:</b>	261.71
<b>CAS:</b>	57338-87-1

## Physical Properties

Property code	Value	Unit	Source
gf	397.65	kJ/mol	Joback Method
hf	182.38	kJ/mol	Joback Method
hfus	34.91	kJ/mol	Joback Method
hvap	81.60	kJ/mol	Joback Method
log10ws	-3.71		Crippen Method
logp	2.610		Crippen Method
mvol	196.820	ml/mol	McGowan Method
pc	2111.94	kPa	Joback Method
tb	836.40	K	Joback Method
tc	1066.73	K	Joback Method
tf	517.51	K	Joback Method
vc	0.780	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	521.44	J/mol×K	836.40	Joback Method
cpg	530.88	J/mol×K	874.79	Joback Method
cpg	539.57	J/mol×K	913.18	Joback Method
cpg	547.55	J/mol×K	951.56	Joback Method
cpg	554.90	J/mol×K	989.95	Joback Method
cpg	561.66	J/mol×K	1028.34	Joback Method
cpg	567.89	J/mol×K	1066.73	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=C57338871&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C57338871&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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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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