

# 2-Chloro-6-fluorobenzyl cyanide

<b>Other names:</b>	2-Chloro-6-fluorophenylacetonitrile Benzeneacetonitrile, 2-chloro-6-fluoro-
<b>Inchi:</b>	InChI=1S/C8H5ClFN/c9-7-2-1-3-8(10)6(7)4-5-11/h1-3H,4H2
<b>InchiKey:</b>	ZGSAFMIRVLOISC-UHFFFAOYSA-N
<b>Formula:</b>	C8H5ClFN
<b>SMILES:</b>	N#CCc1c(F)cccc1Cl
<b>Mol. weight [g/mol]:</b>	169.58
<b>CAS:</b>	75279-55-9

## Physical Properties

Property code	Value	Unit	Source
gf	36.07	kJ/mol	Joback Method
hf	-41.83	kJ/mol	Joback Method
hfus	18.52	kJ/mol	Joback Method
hvap	51.05	kJ/mol	Joback Method
log10ws	-3.16		Crippen Method
logp	2.545		Crippen Method
mcvol	115.210	ml/mol	McGowan Method
pc	3114.04	kPa	Joback Method
tb	557.86	K	Joback Method
tc	784.34	K	Joback Method
tf	326.88	K	Joback Method
vc	0.469	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	229.97	J/mol×K	557.86	Joback Method
cpg	238.45	J/mol×K	595.61	Joback Method
cpg	246.38	J/mol×K	633.35	Joback Method
cpg	253.78	J/mol×K	671.10	Joback Method
cpg	260.68	J/mol×K	708.85	Joback Method
cpg	267.09	J/mol×K	746.59	Joback Method
cpg	273.04	J/mol×K	784.34	Joback Method

# Sources

<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>
<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=C75279559&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C75279559&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>

# 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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