

# loxynil-methyl

<b>Inchi:</b>	InChI=1S/C8H5I2NO/c1-12-8-6(9)2-5(4-11)3-7(8)10/h2-3H,1H3
<b>InchiKey:</b>	LDZMXYUHLHAQAY-UHFFFAOYSA-N
<b>Formula:</b>	C8H5I2NO
<b>SMILES:</b>	COc1c(I)cc(C#N)cc1I
<b>Mol. weight [g/mol]:</b>	384.94
<b>CAS:</b>	3336-40-1

## Physical Properties

Property code	Value	Unit	Source
gf	244.42	kJ/mol	Joback Method
hf	180.07	kJ/mol	Joback Method
hfus	20.86	kJ/mol	Joback Method
hvap	69.30	kJ/mol	Joback Method
log10ws	-4.24		Crippen Method
logp	2.776		Crippen Method
mcvol	158.710	ml/mol	McGowan Method
pc	3135.00	kPa	Joback Method
rinpol	1956.50		NIST Webbook
tb	734.84	K	Joback Method
tc	1023.87	K	Joback Method
tf	447.24	K	Joback Method
vc	0.596	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	285.19	J/molxK	734.84	Joback Method
cpg	292.44	J/molxK	783.01	Joback Method
cpg	299.05	J/molxK	831.18	Joback Method
cpg	305.06	J/molxK	879.36	Joback Method
cpg	310.51	J/molxK	927.53	Joback Method
cpg	315.43	J/molxK	975.70	Joback Method
cpg	319.87	J/molxK	1023.87	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C3336401&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C3336401&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>
<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>

# 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>hvp:</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>rinp:</b>	Non-polar retention indices
<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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