

# 4-Cyanobenzoic acid, dodec-9-ynyl ester

<b>Inchi:</b>	InChI=1S/C20H25NO2/c1-2-3-4-5-6-7-8-9-10-11-16-23-20(22)19-14-12-18(17-21)13-15-
<b>InchiKey:</b>	JPYRZMMDOXDZMV-UHFFFAOYSA-N
<b>Formula:</b>	C20H25NO2
<b>SMILES:</b>	CCC#CCCCCCCCOC(=O)c1ccc(C#N)cc1
<b>Mol. weight [g/mol]:</b>	311.42

## Physical Properties

Property code	Value	Unit	Source
gf	322.36	kJ/mol	Joback Method
hf	-38.69	kJ/mol	Joback Method
hfus	48.62	kJ/mol	Joback Method
hvap	84.84	kJ/mol	Joback Method
log10ws	-6.47		Crippen Method
logp	4.859		Crippen Method
mcvol	269.120	ml/mol	McGowan Method
pc	1433.72	kPa	Joback Method
rinpol	2416.00		NIST Webbook
rinpol	2416.00		NIST Webbook
tb	876.03	K	Joback Method
tc	1094.64	K	Joback Method
tf	597.35	K	Joback Method
vc	1.060	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	807.28	J/molxK	876.03	Joback Method
cpg	821.82	J/molxK	912.46	Joback Method
cpg	835.29	J/molxK	948.90	Joback Method
cpg	847.73	J/molxK	985.33	Joback Method
cpg	859.18	J/molxK	1021.77	Joback Method
cpg	869.69	J/molxK	1058.20	Joback Method
cpg	879.28	J/molxK	1094.64	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=U292453&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U292453&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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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>rinpola:</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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