

# Alpha-cyano-2-norbornaneacetic acid, ethyl ester

Inchi:	InChI=1S/C12H17NO2/c1-2-15-12(14)11(7-13)10-6-8-3-4-9(10)5-8/h8-11H,2-6H2,1H3
InchiKey:	XQMXGJZFEYPEDM-UHFFFAOYSA-N
Formula:	C12H17NO2
SMILES:	CCOC(=O)C(C#N)C1CC2CCC1C2
Mol. weight [g/mol]:	207.27
CAS:	71172-71-9

## Physical Properties

Property code	Value	Unit	Source
gf	48.67	kJ/mol	Joback Method
hf	-257.11	kJ/mol	Joback Method
hfus	22.85	kJ/mol	Joback Method
hvap	61.24	kJ/mol	Joback Method
log10ws	-2.40		Crippen Method
logp	2.125		Crippen Method
mcvol	167.040	ml/mol	McGowan Method
pc	2291.52	kPa	Joback Method
tb	664.97	K	Joback Method
tc	882.80	K	Joback Method
tf	375.27	K	Joback Method
vc	0.656	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	478.72	J/molxK	664.97	Joback Method
cpg	494.49	J/molxK	701.27	Joback Method
cpg	509.24	J/molxK	737.58	Joback Method
cpg	523.03	J/molxK	773.88	Joback Method
cpg	535.92	J/molxK	810.19	Joback Method
cpg	547.96	J/molxK	846.49	Joback Method
cpg	559.22	J/molxK	882.80	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=C71172719&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C71172719&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

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