

# Cyanoacetic acid, tridecyl ester

<b>Inchi:</b>	InChI=1S/C16H29NO2/c1-2-3-4-5-6-7-8-9-10-11-12-15-19-16(18)13-14-17/h2-13,15H2,1
<b>InchiKey:</b>	UVWHRPNFBXRAGB-UHFFFAOYSA-N
<b>Formula:</b>	C16H29NO2
<b>SMILES:</b>	CCCCCCCCCCCCOC(=O)CC#N
<b>Mol. weight [g/mol]:</b>	267.41

## Physical Properties

Property code	Value	Unit	Source
gf	-16.90	kJ/mol	Joback Method
hf	-453.49	kJ/mol	Joback Method
hfus	41.49	kJ/mol	Joback Method
hvap	70.84	kJ/mol	Joback Method
log10ws	-5.25		Crippen Method
logp	4.754		Crippen Method
mvol	245.120	ml/mol	McGowan Method
pc	1338.82	kPa	Joback Method
rinpol	2051.00		NIST Webbook
rinpol	2051.00		NIST Webbook
tb	743.85	K	Joback Method
tc	926.56	K	Joback Method
tf	407.23	K	Joback Method
vc	0.982	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	720.73	J/mol×K	743.85	Joback Method
cpg	736.40	J/mol×K	774.30	Joback Method
cpg	751.27	J/mol×K	804.75	Joback Method
cpg	765.36	J/mol×K	835.20	Joback Method
cpg	778.68	J/mol×K	865.65	Joback Method
cpg	791.25	J/mol×K	896.11	Joback Method
cpg	803.10	J/mol×K	926.56	Joback Method

# Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=U406230&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406230&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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