

# Cyanoacetic acid, octadecyl ester

<b>Inchi:</b>	InChI=1S/C21H39NO2/c1-2-3-4-5-6-7-8-9-10-11-12-13-14-15-16-17-20-24-21(23)18-19-
<b>InchiKey:</b>	NNBNVJGHIBGDAW-UHFFFAOYSA-N
<b>Formula:</b>	C21H39NO2
<b>SMILES:</b>	CCCCCCCCCCCCCCCCCOC(=O)CC#N
<b>Mol. weight [g/mol]:</b>	337.54

## Physical Properties

Property code	Value	Unit	Source
gf	25.20	kJ/mol	Joback Method
hf	-556.69	kJ/mol	Joback Method
hfus	54.44	kJ/mol	Joback Method
hvap	81.97	kJ/mol	Joback Method
log10ws	-7.34		Crippen Method
logp	6.705		Crippen Method
mvol	315.570	ml/mol	McGowan Method
pc	968.68	kPa	Joback Method
rinpol	2565.00		NIST Webbook
rinpol	2565.00		NIST Webbook
tb	858.25	K	Joback Method
tc	1051.47	K	Joback Method
tf	463.58	K	Joback Method
vc	1.262	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	1015.89	J/molxK	858.25	Joback Method
cpg	1033.73	J/molxK	890.45	Joback Method
cpg	1050.52	J/molxK	922.66	Joback Method
cpg	1066.29	J/molxK	954.86	Joback Method
cpg	1081.07	J/molxK	987.06	Joback Method
cpg	1094.90	J/molxK	1019.26	Joback Method
cpg	1107.81	J/molxK	1051.47	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=U406235&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U406235&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>h vap:</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>r in pol:</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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