

# 2-Aminopent-4-enoic acid, N-vinyloxycarbonyl-, octyl ester

<b>Inchi:</b>	InChI=1S/C16H27NO4/c1-4-7-8-9-10-11-13-21-15(18)14(12-5-2)17-16(19)20-6-3/h5-6,14
<b>InchiKey:</b>	NQEXEHOSNJLIME-UHFFFAOYSA-N
<b>Formula:</b>	C16H27NO4
<b>SMILES:</b>	C=CCC(NC(=O)OC=C)C(=O)OCCCCCCCC
<b>Mol. weight [g/mol]:</b>	297.39

## Physical Properties

Property code	Value	Unit	Source
gf	-121.37	kJ/mol	Joback Method
hf	-564.12	kJ/mol	Joback Method
hfus	41.79	kJ/mol	Joback Method
hvap	74.23	kJ/mol	Joback Method
log10ws	-4.73		Crippen Method
logp	3.704		Crippen Method
mvol	252.560	ml/mol	McGowan Method
pc	1529.46	kPa	Joback Method
rinpol	1982.00		NIST Webbook
rinpol	1982.00		NIST Webbook
tb	761.15	K	Joback Method
tc	946.74	K	Joback Method
tf	448.54	K	Joback Method
vc	0.971	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	743.99	J/mol×K	761.15	Joback Method
cpg	759.28	J/mol×K	792.08	Joback Method
cpg	773.69	J/mol×K	823.01	Joback Method
cpg	787.25	J/mol×K	853.95	Joback Method
cpg	799.97	J/mol×K	884.88	Joback Method
cpg	811.86	J/mol×K	915.81	Joback Method
cpg	822.96	J/mol×K	946.74	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=U393212&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U393212&amp;Units=SI</a>
<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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>

# 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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