

# D-(+)-Mannose, aldononitrile, pentaacetate

<b>Inchi:</b>	InChI=1S/C16H21NO10/c1-8(18)23-7-14(25-10(3)20)16(27-12(5)22)15(26-11(4)21)13(6
<b>InchiKey:</b>	INCBLRCTSZYSJE-UHFFFAOYSA-N
<b>Formula:</b>	C16H21NO10
<b>SMILES:</b>	CC(=O)OCC(OC(C)=O)C(OC(C)=O)C(OC(C)=O)C(C#N)OC(C)=O
<b>Mol. weight [g/mol]:</b>	387.34

## Physical Properties

Property code	Value	Unit	Source
gf	-962.34	kJ/mol	Joback Method
hf	-1453.81	kJ/mol	Joback Method
hfus	38.55	kJ/mol	Joback Method
hvap	105.92	kJ/mol	Joback Method
log10ws	-1.15		Crippen Method
logp	-0.200		Crippen Method
mcvol	274.880	ml/mol	McGowan Method
pc	1578.46	kPa	Joback Method
rinsol	1937.80		NIST Webbook
tb	1047.25	K	Joback Method
tc	1282.15	K	Joback Method
tf	635.87	K	Joback Method
vc	1.054	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	870.07	J/mol×K	1047.25	Joback Method
cpg	875.40	J/mol×K	1086.40	Joback Method
cpg	878.69	J/mol×K	1125.55	Joback Method
cpg	879.90	J/mol×K	1164.70	Joback Method
cpg	878.96	J/mol×K	1203.85	Joback Method
cpg	875.84	J/mol×K	1243.00	Joback Method
cpg	870.46	J/mol×K	1282.15	Joback Method

# Sources

<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>
<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=U380434&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=U380434&amp;Units=SI</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>mccvol:</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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