

# Panaxjapyne A

<b>Inchi:</b>	InChI=1S/C17H26O/c1-3-5-6-7-8-9-10-11-12-13-14-15-16-17(18)4-2/h10-11,17-18H,3-9,
<b>InchiKey:</b>	PROIGOAKZLZHQV-KHPPLWFESA-N
<b>Formula:</b>	C17H26O
<b>SMILES:</b>	CCCCCCCC=CCC#CC#CC(O)CC
<b>Mol. weight [g/mol]:</b>	246.39
<b>CAS:</b>	1242413-82-6

## Physical Properties

Property code	Value	Unit	Source
gf	438.82	kJ/mol	Joback Method
hf	110.10	kJ/mol	Joback Method
hfus	46.80	kJ/mol	Joback Method
hvap	73.99	kJ/mol	Joback Method
log10ws	-5.76		Crippen Method
logp	4.071		Crippen Method
mcvol	234.760	ml/mol	McGowan Method
pc	1768.38	kPa	Joback Method
rinpol	1993.80		NIST Webbook
tb	702.26	K	Joback Method
tc	894.78	K	Joback Method
tf	534.29	K	Joback Method
vc	0.904	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	640.39	J/molxK	702.26	Joback Method
cpg	656.42	J/molxK	734.35	Joback Method
cpg	671.66	J/molxK	766.43	Joback Method
cpg	686.15	J/molxK	798.52	Joback Method
cpg	699.95	J/molxK	830.61	Joback Method
cpg	713.08	J/molxK	862.70	Joback Method
cpg	725.59	J/molxK	894.78	Joback Method

# Sources

<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=C1242413826&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1242413826&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>

# 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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