

# 3-Diethylamino-5,7-dimethyloctyne-1

<b>Inchi:</b>	InChI=1S/C14H27N/c1-7-14(15(8-2)9-3)11-13(6)10-12(4)5/h1,12-14H,8-11H2,2-6H3
<b>InchiKey:</b>	XLSSYWHORCDDFFA-UHFFFAOYSA-N
<b>Formula:</b>	C14H27N
<b>SMILES:</b>	C#CC(CC(C)CC(C)C)N(CC)CC
<b>Mol. weight [g/mol]:</b>	209.37
<b>CAS:</b>	116595-26-7

## Physical Properties

Property code	Value	Unit	Source
gf	393.53	kJ/mol	Joback Method
hf	11.30	kJ/mol	Joback Method
hfus	27.44	kJ/mol	Joback Method
hvap	47.50	kJ/mol	Joback Method
log10ws	-3.68		Crippen Method
logp	3.402		Crippen Method
mcvol	209.500	ml/mol	McGowan Method
pc	1747.74	kPa	Joback Method
tb	520.96	K	Joback Method
tc	698.09	K	Joback Method
tf	281.98	K	Joback Method
vc	0.781	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	505.31	J/molxK	520.96	Joback Method
cpg	524.36	J/molxK	550.48	Joback Method
cpg	542.51	J/molxK	580.00	Joback Method
cpg	559.81	J/molxK	609.53	Joback Method
cpg	576.29	J/molxK	639.05	Joback Method
cpg	591.98	J/molxK	668.57	Joback Method
cpg	606.90	J/molxK	698.09	Joback Method

# Sources

<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=C116595267&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C116595267&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.chemeo.com/doc/models/crippen_log10ws">https://www.chemeo.com/doc/models/crippen_log10ws</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>m cvol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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