

# cis 2-Hexenoic acid amide

<b>Inchi:</b>	InChI=1S/C6H11NO/c1-2-3-4-5-6(7)8/h4-5H,2-3H2,1H3,(H2,7,8)/b5-4-
<b>InchiKey:</b>	BZEUYEFVVDTL0D-PLNGDYQASA-N
<b>Formula:</b>	C6H11NO
<b>SMILES:</b>	CCCC=CC(N)=O
<b>Mol. weight [g/mol]:</b>	113.16
<b>CAS:</b>	820-99-5

## Physical Properties

Property code	Value	Unit	Source
gf	17.39	kJ/mol	Joback Method
hf	-128.74	kJ/mol	Joback Method
hfus	18.29	kJ/mol	Joback Method
hvap	46.30	kJ/mol	Joback Method
log10ws	-1.40		Crippen Method
logp	0.828		Crippen Method
mcvol	102.650	ml/mol	McGowan Method
pc	3801.00	kPa	Joback Method
tb	467.24	K	Joback Method
tc	667.96	K	Joback Method
tf	285.49	K	Joback Method
vc	0.387	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	257.87	J/molxK	634.51	Joback Method
cpg	211.82	J/molxK	467.24	Joback Method
cpg	222.09	J/molxK	500.69	Joback Method
cpg	231.80	J/molxK	534.15	Joback Method
cpg	240.99	J/molxK	567.60	Joback Method
cpg	249.67	J/molxK	601.06	Joback Method
cpg	265.63	J/molxK	667.96	Joback Method
hsubt	80.00	kJ/mol	328.00	NIST Webbook
hvapt	61.70	kJ/mol	363.00	NIST Webbook

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci9903071">http://pubs.acs.org/doi/abs/10.1021/ci9903071</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=C820995&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C820995&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>hsubt:</b>	Enthalpy of sublimation at a given temperature
<b>hvap:</b>	Enthalpy of vaporization at standard conditions
<b>hvapt:</b>	Enthalpy of vaporization at a given temperature
<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>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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