

# Isoquinoline, decahydro-

<b>Other names:</b>	Decahydroisoquinoline Perhydroisoquinoline Perhydroisoquinoline,c&t
<b>Inchi:</b>	InChI=1S/C9H17N/c1-2-4-9-7-10-6-5-8(9)3-1/h8-10H,1-7H2
<b>InchiKey:</b>	NENLYAQP NATJSU-UHFFFAOYSA-N
<b>Formula:</b>	C9H17N
<b>SMILES:</b>	C1CCC2CNCCC2C1
<b>Mol. weight [g/mol]:</b>	139.24
<b>CAS:</b>	6329-61-9

## Physical Properties

Property code	Value	Unit	Source
gf	185.71	kJ/mol	Joback Method
hf	-70.32	kJ/mol	Joback Method
hfus	16.53	kJ/mol	Joback Method
hvap	42.90	kJ/mol	Joback Method
log10ws	-2.09		Crippen Method
logp	1.786		Crippen Method
mcvol	125.930	ml/mol	McGowan Method
pc	3472.45	kPa	Joback Method
ripol	1560.00		NIST Webbook
ripol	1560.00		NIST Webbook
ripol	1520.00		NIST Webbook
tb	484.43	K	Joback Method
tc	716.50	K	Joback Method
tf	318.02	K	Joback Method
vc	0.459	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	289.06	J/mol×K	484.43	Joback Method
cpg	310.41	J/mol×K	523.11	Joback Method
cpg	330.45	J/mol×K	561.79	Joback Method

cpg	349.23	J/mol×K	600.46	Joback Method
cpg	366.80	J/mol×K	639.14	Joback Method
cpg	383.22	J/mol×K	677.82	Joback Method
cpg	398.52	J/mol×K	716.50	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=C6329619&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C6329619&amp;Units=SI</a>
<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>

## 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>ripol:</b>	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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