

# 3-ethyl-octahydroindole

<b>Inchi:</b>	InChI=1S/C10H19N/c1-2-8-7-11-10-6-4-3-5-9(8)10/h8-11H,2-7H2,1H3
<b>InchiKey:</b>	POQZASNPVNSKNG-UHFFFAOYSA-N
<b>Formula:</b>	C10H19N
<b>SMILES:</b>	CCC1CNC2CCCCC12
<b>Mol. weight [g/mol]:</b>	153.26

## Physical Properties

Property code	Value	Unit	Source
gf	198.52	kJ/mol	Joback Method
hf	-105.14	kJ/mol	Joback Method
hfus	22.29	kJ/mol	Joback Method
hvap	44.64	kJ/mol	Joback Method
log10ws	-2.62		Crippen Method
logp	2.175		Crippen Method
mcvol	140.020	ml/mol	McGowan Method
pc	2918.68	kPa	Joback Method
ripol	1308.00		NIST Webbook
ripol	1308.00		NIST Webbook
ripol	1326.00		NIST Webbook
ripol	1513.00		NIST Webbook
ripol	1523.00		NIST Webbook
tb	498.37	K	Joback Method
tc	717.72	K	Joback Method
tf	328.57	K	Joback Method
vc	0.521	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	336.39	J/mol×K	498.37	Joback Method
cpg	357.70	J/mol×K	534.93	Joback Method
cpg	377.78	J/mol×K	571.49	Joback Method
cpg	396.69	J/mol×K	608.05	Joback Method
cpg	414.48	J/mol×K	644.61	Joback Method

cpg	431.18	J/mol×K	681.16	Joback Method
cpg	446.85	J/mol×K	717.72	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=R135167&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R135167&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>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>rinpolar:</b>	Non-polar retention indices
<b>ripolar:</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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