

# 4-Isopropyl-piperidine

<b>Inchi:</b>	InChI=1S/C8H17N/c1-7(2)8-3-5-9-6-4-8/h7-9H,3-6H2,1-2H3
<b>InchiKey:</b>	YBPWIUSXQXYTSR-UHFFFAOYSA-N
<b>Formula:</b>	C8H17N
<b>SMILES:</b>	CC(C)C1CCNCC1
<b>Mol. weight [g/mol]:</b>	127.23

## Physical Properties

Property code	Value	Unit	Source
gf	126.20	kJ/mol	Joback Method
hf	-121.60	kJ/mol	Joback Method
hfus	14.38	kJ/mol	Joback Method
hvap	40.20	kJ/mol	Joback Method
log10ws	-1.77		Crippen Method
logp	1.642		Crippen Method
mcvol	122.700	ml/mol	McGowan Method
pc	3272.78	kPa	Joback Method
rinsol	1012.00		NIST Webbook
tb	450.10	K	Joback Method
tc	663.96	K	Joback Method
tf	277.33	K	Joback Method
vc	0.448	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	258.00	J/molxK	450.10	Joback Method
cpg	276.21	J/molxK	485.74	Joback Method
cpg	293.54	J/molxK	521.39	Joback Method
cpg	310.00	J/molxK	557.03	Joback Method
cpg	325.61	J/molxK	592.67	Joback Method
cpg	340.39	J/molxK	628.32	Joback Method
cpg	354.35	J/molxK	663.96	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=R405926&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R405926&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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<b>rinpol:</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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