

# isoamyl-n-hexyl-amine

<b>Inchi:</b>	InChI=1S/C11H25N/c1-4-5-6-7-9-12-10-8-11(2)3/h11-12H,4-10H2,1-3H3
<b>InchiKey:</b>	PQLZIHKBARHEC-UHFFFAOYSA-N
<b>Formula:</b>	C11H25N
<b>SMILES:</b>	CCCCCNCCC(C)C
<b>Mol. weight [g/mol]:</b>	171.32

## Physical Properties

Property code	Value	Unit	Source
gf	128.69	kJ/mol	Joback Method
hf	-222.18	kJ/mol	Joback Method
hfus	25.82	kJ/mol	Joback Method
hvap	46.13	kJ/mol	Joback Method
log10ws	-3.37		Crippen Method
logp	3.202		Crippen Method
mcvol	175.830	ml/mol	McGowan Method
pc	1970.05	kPa	Joback Method
rinpol	1203.00		NIST Webbook
tb	500.81	K	Joback Method
tc	669.39	K	Joback Method
tf	251.39	K	Joback Method
vc	0.680	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	415.58	J/mol×K	500.81	Joback Method
cpg	432.13	J/mol×K	528.91	Joback Method
cpg	448.02	J/mol×K	557.00	Joback Method
cpg	463.26	J/mol×K	585.10	Joback Method
cpg	477.87	J/mol×K	613.19	Joback Method
cpg	491.87	J/mol×K	641.29	Joback Method
cpg	505.27	J/mol×K	669.39	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=R521776&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R521776&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>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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