

# Isohexylamine

<b>Inchi:</b>	InChI=1S/C6H15N/c1-6(2)4-3-5-7/h6H,3-5,7H2,1-2H3
<b>InchiKey:</b>	QVIAMKXOQGCV-UHFFFAOYSA-N
<b>Formula:</b>	C6H15N
<b>SMILES:</b>	CC(C)CCCN
<b>Mol. weight [g/mol]:</b>	101.19

## Physical Properties

Property code	Value	Unit	Source
gf	63.65	kJ/mol	Joback Method
hf	-138.66	kJ/mol	Joback Method
hfus	12.97	kJ/mol	Joback Method
hvap	39.20	kJ/mol	Joback Method
log10ws	-1.53		Crippen Method
logp	1.381		Crippen Method
mcvol	105.380	ml/mol	McGowan Method
pc	3345.11	kPa	Joback Method
tb	408.77	K	Joback Method
tc	592.91	K	Joback Method
tf	225.64	K	Joback Method
vc	0.395	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	211.01	J/molxK	408.77	Joback Method
cpg	222.78	J/molxK	439.46	Joback Method
cpg	234.07	J/molxK	470.15	Joback Method
cpg	244.89	J/molxK	500.84	Joback Method
cpg	255.25	J/molxK	531.53	Joback Method
cpg	265.17	J/molxK	562.22	Joback Method
cpg	274.66	J/molxK	592.91	Joback Method

# Sources

<b>KDB:</b>	<a href="https://www.cheric.org/files/research/kdb/mol/mol1393.mol">https://www.cheric.org/files/research/kdb/mol/mol1393.mol</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>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>
<b>Joback Method:</b>	<a href="https://en.wikipedia.org/wiki/Joback_method">https://en.wikipedia.org/wiki/Joback_method</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>mccvol:</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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