

# 3-Isopropoxypropylamine

<b>Other names:</b>	3-Isopropoxy-n-propylamine 1-Propanamine, 3-(1-methylethoxy)- Isopropoxypropylamine Propylamine, 3-isopropoxy- 3-(1-Methylethoxy)-1-propanamine 3-Isopropoxy-1-propylamine
<b>Inchi:</b>	InChI=1S/C6H15NO/c1-6(2)8-5-3-4-7/h6H,3-5,7H2,1-2H3
<b>InchiKey:</b>	VHYUNSUGCNKWSO-UHFFFAOYSA-N
<b>Formula:</b>	C6H15NO
<b>SMILES:</b>	CC(C)OCCCN
<b>Mol. weight [g/mol]:</b>	117.19
<b>CAS:</b>	2906-12-9

## Physical Properties

Property code	Value	Unit	Source
gf	-41.35	kJ/mol	Joback Method
hf	-270.88	kJ/mol	Joback Method
hfus	14.16	kJ/mol	Joback Method
hvap	41.61	kJ/mol	Joback Method
log10ws	-0.97		Crippen Method
logp	0.760		Crippen Method
mcvol	111.250	ml/mol	McGowan Method
pc	3280.28	kPa	Joback Method
tb	431.19	K	Joback Method
tc	614.99	K	Joback Method
tf	247.87	K	Joback Method
vc	0.412	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	234.15	J/mol×K	431.19	Joback Method
cpg	245.64	J/mol×K	461.82	Joback Method
cpg	256.73	J/mol×K	492.46	Joback Method

cpg	267.42	J/mol×K	523.09	Joback Method
cpg	277.70	J/mol×K	553.72	Joback Method
cpg	287.59	J/mol×K	584.35	Joback Method
cpg	297.08	J/mol×K	614.99	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	351.70	K	11.00	NIST Webbook

## Sources

<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>
<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=C2906129&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C2906129&amp;Units=SI</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>tb:</b>	Normal Boiling Point Temperature
<b>tbrp:</b>	Boiling point at reduced pressure
<b>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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