

# Isobutylcarbamate, N-sec.-butyl

<b>Inchi:</b>	InChI=1S/C13H27NO2/c1-7-11(5)14(12(6)8-2)13(15)16-9-10(3)4/h10-12H,7-9H2,1-6H3
<b>InchiKey:</b>	XFSXTCIIMPNGHP-UHFFFAOYSA-N
<b>Formula:</b>	C13H27NO2
<b>SMILES:</b>	CCC(C)N(C(=O)OCC(C)C)C(C)CC
<b>Mol. weight [g/mol]:</b>	229.36

## Physical Properties

Property code	Value	Unit	Source
gf	-71.88	kJ/mol	Joback Method
hf	-504.76	kJ/mol	Joback Method
hfus	24.66	kJ/mol	Joback Method
hvap	54.57	kJ/mol	Joback Method
log10ws	-3.66		Crippen Method
logp	3.678		Crippen Method
mvol	211.450	ml/mol	McGowan Method
pc	1739.01	kPa	Joback Method
rpol	1207.00		NIST Webbook
tb	584.25	K	Joback Method
tc	760.47	K	Joback Method
tf	295.90	K	Joback Method
vc	0.787	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	553.81	J/mol×K	584.25	Joback Method
cpg	571.55	J/mol×K	613.62	Joback Method
cpg	588.49	J/mol×K	642.99	Joback Method
cpg	604.65	J/mol×K	672.36	Joback Method
cpg	620.05	J/mol×K	701.73	Joback Method
cpg	634.70	J/mol×K	731.10	Joback Method
cpg	648.62	J/mol×K	760.47	Joback Method

# Sources

<b>Crippen Method:</b>	<a href="http://pubs.acs.org/doi/abs/10.1021/ci990307I">http://pubs.acs.org/doi/abs/10.1021/ci990307I</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=R392726&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=R392726&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>mccvol:</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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