

# Propane, 2-isocyanato-2-methyl-

<b>Other names:</b>	Isocyanic acid, tert-butyl ester t-butylisocyanate tert-Butyl Isocyanate 1,1-Dimethylethyl isocyanate t-C <sub>4</sub> H <sub>9</sub> NCO UN 2484
<b>Inchi:</b>	InChI=1S/C <sub>5</sub> H <sub>9</sub> NO/c1-5(2,3)6-4-7/h1-3H3
<b>InchiKey:</b>	MGOLNIXAPIAKFM-UHFFFAOYSA-N
<b>Formula:</b>	C <sub>5</sub> H <sub>9</sub> NO
<b>SMILES:</b>	CC(C)(C)N=C=O
<b>Mol. weight [g/mol]:</b>	99.13
<b>CAS:</b>	1609-86-5

## Physical Properties

Property code	Value	Unit	Source
hf	-160.69	kJ/mol	Joback Method
hvap	34.96	kJ/mol	Joback Method
ie	10.14	eV	NIST Webbook
ie	9.57	eV	NIST Webbook
log10ws	-5.52		Crippen Method
logp	1.121		Crippen Method
mcvol	88.560	ml/mol	McGowan Method
pc	3881.95	kPa	Joback Method
tb	377.24	K	Joback Method
tc	568.26	K	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=C1609865&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C1609865&amp;Units=SI</a>
<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>

# Legend

<b>hf:</b>	Enthalpy of formation at standard conditions
<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>ie:</b>	Ionization energy
<b>log<sub>10</sub>ws:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</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>tc:</b>	Critical Temperature

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