

# 2-N-Carbobutoxyphenyl isocyanate

<b>Other names:</b>	2-Butoxycarbonylphenyl isocyanate 4-n-Butoxycarbonylphenyl isocyanate
<b>Inchi:</b>	InChI=1S/C12H13NO3/c1-2-3-8-16-12(15)10-6-4-5-7-11(10)13-9-14/h4-7H,2-3,8H2,1H3
<b>InchiKey:</b>	QNWQMUCMHVKVGU-UHFFFAOYSA-N
<b>Formula:</b>	C12H13NO3
<b>SMILES:</b>	CCCCOC(=O)c1ccccc1N=C=O
<b>Mol. weight [g/mol]:</b>	219.24
<b>CAS:</b>	51310-19-1

## Physical Properties

Property code	Value	Unit	Source
hf	-316.16	kJ/mol	Joback Method
hvac	63.93	kJ/mol	Joback Method
log10ws	-7.45		Crippen Method
logp	2.611		Crippen Method
mccvol	170.870	ml/mol	McGowan Method
pc	2673.54	kPa	Joback Method
tb	648.58	K	Joback Method
tc	861.62	K	Joback Method

## Sources

<b>NIST Webbook:</b>	<a href="http://webbook.nist.gov/cgi/cbook.cgi?ID=C51310191&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C51310191&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>
<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>

## Legend

hf: Enthalpy of formation at standard conditions

<b>h<sub>vap</sub>:</b>	Enthalpy of vaporization at standard conditions
<b>log<sub>10</sub>w<sub>s</sub>:</b>	Log10 of Water solubility in mol/l
<b>log<sub>p</sub>:</b>	Octanol/Water partition coefficient
<b>mc<sub>vol</sub>:</b>	McGowan's characteristic volume
<b>p<sub>c</sub>:</b>	Critical Pressure
<b>t<sub>b</sub>:</b>	Normal Boiling Point Temperature
<b>t<sub>c</sub>:</b>	Critical Temperature

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