

# 2-[1-Naphthyl]-3-oxobutyronitrile

<b>Inchi:</b>	InChI=1S/C14H11NO/c1-10(16)14(9-15)13-8-4-6-11-5-2-3-7-12(11)13/h2-8,14H,1H3
<b>InchiKey:</b>	XTTACCFJXCXIIIH-UHFFFAOYSA-N
<b>Formula:</b>	C14H12O
<b>SMILES:</b>	CC(=O)C(C#N)c1cccc2ccccc12
<b>Mol. weight [g/mol]:</b>	196.24
<b>CAS:</b>	31573-38-3

## Physical Properties

Property code	Value	Unit	Source
gf	278.25	kJ/mol	Joback Method
hf	130.86	kJ/mol	Joback Method
hfus	22.27	kJ/mol	Joback Method
hvap	68.17	kJ/mol	Joback Method
log10ws	-4.03		Crippen Method
logp	3.036		Crippen Method
mvol	167.850	ml/mol	McGowan Method
pc	2616.41	kPa	Joback Method
tb	725.87	K	Joback Method
tc	971.64	K	Joback Method
tf	419.10	K	Joback Method
vc	0.659	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	430.69	J/mol×K	725.87	Joback Method
cpg	442.64	J/mol×K	766.83	Joback Method
cpg	453.64	J/mol×K	807.79	Joback Method
cpg	463.78	J/mol×K	848.75	Joback Method
cpg	473.16	J/mol×K	889.72	Joback Method
cpg	481.85	J/mol×K	930.68	Joback Method
cpg	489.97	J/mol×K	971.64	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	417.00 ± 1.00	K	0.01	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=C31573383&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C31573383&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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