

# O-nitro carbanilic acid, bornyl ester

<b>Inchi:</b>	InChI=1S/C17H22N2O4/c1-16(2)11-8-9-17(16,3)14(10-11)23-15(20)18-12-6-4-5-7-13(12)
<b>InchiKey:</b>	VBVDYKQSBWRJID-UHFFFAOYSA-N
<b>Formula:</b>	C17H22N2O4
<b>SMILES:</b>	CC1(C)C2CCC1(C)C(OC(=O)Nc1ccccc1[N+](=O)[O-])C2
<b>Mol. weight [g/mol]:</b>	318.37
<b>CAS:</b>	93437-07-1

## Physical Properties

Property code	Value	Unit	Source
gf	169.06	kJ/mol	Joback Method
hf	-242.00	kJ/mol	Joback Method
hfus	36.40	kJ/mol	Joback Method
hvap	85.63	kJ/mol	Joback Method
log10ws	-5.33		Crippen Method
logp	4.358		Crippen Method
mcvol	239.750	ml/mol	McGowan Method
pc	2155.30	kPa	Joback Method
tb	907.21	K	Joback Method
tc	1160.91	K	Joback Method
tf	660.40	K	Joback Method
vc	0.920	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	804.86	J/molxK	907.21	Joback Method
cpg	827.00	J/molxK	949.49	Joback Method
cpg	850.06	J/molxK	991.78	Joback Method
cpg	874.43	J/molxK	1034.06	Joback Method
cpg	900.50	J/molxK	1076.35	Joback Method
cpg	928.68	J/molxK	1118.63	Joback Method
cpg	959.34	J/molxK	1160.91	Joback Method

# Sources

<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=C93437071&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C93437071&amp;Units=SI</a>
<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>

# 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>hvac:</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>mccol:</b>	McGowan's characteristic volume
<b>pc:</b>	Critical Pressure
<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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