

# 4-Benzoxazone, 2-(2'-dimethylamino-1',1'-dimethylethyl)-

**Inchi:** InChI=1S/C14H20N2O2/c1-14(2,9-16(3)4)13-15-12(17)10-7-5-6-8-11(10)18-13/h5-8,13H

**InchiKey:** HRIYSWRBGZMFCC-UHFFFAOYSA-N

**Formula:** C14H20N2O2

**SMILES:** CN(C)CC(C)(C)C1NC(=O)c2ccccc2O1

**Mol. weight [g/mol]:** 248.32

## Physical Properties

Property code	Value	Unit	Source
gf	211.05	kJ/mol	Joback Method
hf	-213.70	kJ/mol	Joback Method
hfus	34.39	kJ/mol	Joback Method
hvap	66.04	kJ/mol	Joback Method
log10ws	-2.86		Crippen Method
logp	1.723		Crippen Method
mcvol	200.900	ml/mol	McGowan Method
pc	2443.48	kPa	Joback Method
tb	714.92	K	Joback Method
tc	953.44	K	Joback Method
tf	535.61	K	Joback Method
vc	0.733	m3/kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	588.49	J/molxK	714.92	Joback Method
cpg	606.64	J/molxK	754.67	Joback Method
cpg	623.43	J/molxK	794.43	Joback Method
cpg	638.91	J/molxK	834.18	Joback Method
cpg	653.15	J/molxK	873.94	Joback Method
cpg	666.23	J/molxK	913.69	Joback Method
cpg	678.20	J/molxK	953.44	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=B6000678&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=B6000678&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>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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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