

# 2-Butene, 2-nitro-

<b>Other names:</b>	2-Nitro-2-butene
<b>Inchi:</b>	InChI=1S/C4H7NO2/c1-3-4(2)5(6)7/h3H,1-2H3/b4-3+
<b>InchiKey:</b>	DAHZYRVPEHDLPG-ONEGZZNKSA-N
<b>Formula:</b>	C4H7NO2
<b>SMILES:</b>	CC=C(C)[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	101.10
<b>CAS:</b>	4812-23-1

## Physical Properties

Property code	Value	Unit	Source
gf	90.02	kJ/mol	Joback Method
hf	-29.22	kJ/mol	Joback Method
hfus	16.37	kJ/mol	Joback Method
hvap	41.13	kJ/mol	Joback Method
log10ws	-1.93		Crippen Method
logp	1.187		Crippen Method
mcvol	80.340	ml/mol	McGowan Method
pc	4255.16	kPa	Joback Method
tb	446.80	K	Joback Method
tc	669.05	K	Joback Method
tf	259.41	K	Joback Method
vc	0.323	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	153.53	J/molxK	446.80	Joback Method
cpg	162.35	J/molxK	483.84	Joback Method
cpg	170.61	J/molxK	520.88	Joback Method
cpg	178.34	J/molxK	557.93	Joback Method
cpg	185.56	J/molxK	594.97	Joback Method
cpg	192.32	J/molxK	632.01	Joback Method
cpg	198.65	J/molxK	669.05	Joback Method

# 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.cheméo.com/doc/models/crippen_log10ws">https://www.cheméo.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=C4812231&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C4812231&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>tc:</b>	Critical Temperature
<b>tf:</b>	Normal melting (fusion) point
<b>vc:</b>	Critical Volume

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