

# Ethanol, 2-nitro-

<b>Other names:</b>	«beta»-Nitroethanol 2-Nitroethanol «beta»-Nitroethyl alcohol Nitroethanol
<b>Inchi:</b>	InChI=1S/C2H5NO3/c4-2-1-3(5)6/h4H,1-2H2
<b>InchiKey:</b>	KIPMDPDAFINLIV-UHFFFAOYSA-N
<b>Formula:</b>	C2H5NO3
<b>SMILES:</b>	O=[N+](O)CCO
<b>Mol. weight [g/mol]:</b>	91.07
<b>CAS:</b>	625-48-9

## Physical Properties

Property code	Value	Unit	Source
chl	-921.32	kJ/mol	NIST Webbook
chl	-1210.00	kJ/mol	NIST Webbook
chl	-1151.00	kJ/mol	NIST Webbook
gf	-135.31	kJ/mol	Joback Method
hf	-247.60	kJ/mol	Joback Method
hfl	-351.00	kJ/mol	NIST Webbook
hfus	16.39	kJ/mol	Joback Method
hvap	53.32	kJ/mol	Joback Method
log10ws	-7.51e-03		Crippen Method
logp	-0.745		Crippen Method
mcvol	62.330	ml/mol	McGowan Method
pc	5862.92	kPa	Joback Method
rinpol	658.00		NIST Webbook
rinpol	658.00		NIST Webbook
ripol	2045.00		NIST Webbook
ripol	2045.00		NIST Webbook
tb	489.18	K	Joback Method
tc	689.04	K	Joback Method
tf	316.73	K	Joback Method
vc	0.248	m3/kmol	Joback Method

# Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	130.46	J/mol×K	489.18	Joback Method
cpg	135.90	J/mol×K	522.49	Joback Method
cpg	141.07	J/mol×K	555.80	Joback Method
cpg	145.95	J/mol×K	589.11	Joback Method
cpg	150.58	J/mol×K	622.42	Joback Method
cpg	154.95	J/mol×K	655.73	Joback Method
cpg	159.07	J/mol×K	689.04	Joback Method

# Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	467.20	K	102.00	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=C625489&amp;Units=SI">http://webbook.nist.gov/cgi/cbook.cgi?ID=C625489&amp;Units=SI</a>

## Legend

<b>chl:</b>	Standard liquid enthalpy of combustion
<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>hfl:</b>	Liquid phase 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>rinpol:</b>	Non-polar retention indices
<b>ripol:</b>	Polar retention indices
<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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