

# 1,2-Dinitroethane

<b>Inchi:</b>	InChI=1S/C2H4N2O4/c5-3(6)1-2-4(7)8/h1-2H2
<b>InchiKey:</b>	UXGRXJVMQSSUGS-UHFFFAOYSA-N
<b>Formula:</b>	C2H4N2O4
<b>SMILES:</b>	O=[N+]([O-])CC[N+](=O)[O-]
<b>Mol. weight [g/mol]:</b>	120.06
<b>CAS:</b>	7570-26-5

## Physical Properties

Property code	Value	Unit	Source
chs	-1185.40	kJ/mol	NIST Webbook
chs	-1183.00 ± 1.20	kJ/mol	NIST Webbook
chs	-1180.00 ± 0.80	kJ/mol	NIST Webbook
gf	37.06	kJ/mol	Joback Method
hf	-106.13	kJ/mol	Joback Method
hfs	-176.00 ± 1.20	kJ/mol	NIST Webbook
hfs	-179.00 ± 0.80	kJ/mol	NIST Webbook
hfs	-173.30	kJ/mol	NIST Webbook
hfus	23.66	kJ/mol	Joback Method
hvap	53.23	kJ/mol	Joback Method
log10ws	-0.83		Crippen Method
logp	-0.460		Crippen Method
mcvol	73.880	ml/mol	McGowan Method
pc	5205.63	kPa	Joback Method
tb	548.84	K	Joback Method
tc	796.41	K	Joback Method
tf	399.52	K	Joback Method
vc	0.311	m <sup>3</sup> /kmol	Joback Method

## Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	163.28	J/mol×K	548.84	Joback Method
cpg	170.21	J/mol×K	590.10	Joback Method
cpg	176.63	J/mol×K	631.36	Joback Method

cpg	182.56	J/mol×K	672.62	Joback Method
cpg	188.03	J/mol×K	713.89	Joback Method
cpg	193.06	J/mol×K	755.15	Joback Method
cpg	197.66	J/mol×K	796.41	Joback Method

## Pressure Dependent Properties

Property code	Value	Unit	Pressure [kPa]	Source
tbrp	368.20	K	0.70	NIST Webbook

## 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=C7570265&amp;Units=SI&amp;Mask=3FFF">http://webbook.nist.gov/cgi/cbook.cgi?ID=C7570265&amp;Units=SI&amp;Mask=3FFF</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>chs:</b>	Standard solid 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>hfs:</b>	Solid 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>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

**vc:** Critical Volume

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